ADVANCES IN MATHEMATICS 79, 213–270 (1990)

An Atomic Energy Lower Bound That Agrees with Scott's Correction

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Communicated by Gian-Carlo Rota

In this paper, we prove that the energy of an atom with nuclear charge Z is greater than $-C_{\mathrm{TF}}Z^{7/3}+(q/8)Z^2+O(Z^{17/9}\log Z)$ atomic units as $Z\to\infty$. q is the number of spin states ($q=2$ for electrons) and C_{TF} is the Thomas–Fermi constant for such systems.

0. INTRODUCTION

In their efforts to understand the statistical properties of the electron density in atoms and molecules, Thomas and Fermi independently invented Thomas–Fermi, or T-F, theory in 1927. In its modern formulation, T-F theory is the analysis of the electron density function $p(x)$, $x\in\mathbb{R}^3$, which maximizes the T-F energy functional. For an atom of charge Z, this functional equals

$$E_{\mathrm{TF}}(Z,\rho)=\frac{3}{5}\gamma\int p^{5/3}(x)\,dx-Z\int p(x)\,|x|^{-1}\,dx$$

$$+\frac{1}{2}\iint|x-y|^{-1}\,p(x)\,p(y)\,dx\,dy$$

with $\gamma=(6\pi^2/q)^{2/3}$, and q the number of physical spin states. For electrons, $q=2$. The three terms model the kinetic energy, the electrons' attraction to the nucleus, and their repulsion from the other electrons, respectively. We will refer to them as K, $-A$, and R, respectively. The energy is expressed in Hartree's atomic units. That is, $K/2m=1$. The Thomas–Fermi energy is

$$E_{\mathrm{TF}}(Z)=\min\{E_{\mathrm{TF}}(Z,p)\,|\,p\geqslant 0,\,p\in L'\cap L^{5/3}\}.$$

The functional $E_{\mathrm{TF}}(Z,p)$ always attains its minimum at a unique $p_Z(x)$ with $\int p_Z(x)\,dx=Z$. By rescaling, it is easy to see that $p_Z(x)=Z^2p(Z^{1/3}x)$, where p is the minimizer for $Z=1$.

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Associated to $E_{\mathrm{TF}}(1, p)$ is the variational equation

$$\gamma p^{2/3}(x) = |x|^{-1} - \int |x-y|^{-1} p(y)\, dy.$$

Quantum mechanical convention (see [1]) has the right-hand side written $y(|x|\,\gamma^{-1})|x|^{-1}$, where y satisfies

$$y''(r) = y^{3/2}(r)\, r^{-1/2}, \qquad r > 0$$
$$y(0) = 1, \qquad \lim_{r \to \infty} y(r) = 0.$$

See [2] for an analysis of this solution. For the discussion which follows, we will need some facts about y that are presented in [2]. First, there is a unique boundary value $y'(0) = -\omega$, $\omega \approx 1.5888...$, which gives the desired behavior at infinity. Near $r = 0$, y can be represented

$$y(r) = 1 - \omega r + 4/3\, r^{3/2} + O(r^{5/2}) \tag{0.1}$$

with derivatives having the corresponding form as $r \to \infty$,

$$y(r) = 144^{r-3}\left(1 + \sum_{n=1}^{\infty} c_n r^{-n\tau}\right), \qquad \tau = \frac{1}{2}(\sqrt{73} - 7). \tag{0.2}$$

This sum converges. The necessary fact for us is that given $\varepsilon > 0$ we can pick $\bar{r}(\varepsilon)$ so that if $r > \bar{r}(\varepsilon)$, then $y(r)$ and its first three derivatives agree with $155x^{-3}$ and its first three derivatives within a factor $1 \pm \varepsilon$. The solution y is C^{∞}, strictly positive, monotone decreasing, and convex.

Reference [3] is a thorough discussion of p and it properties. The scaling $p_Z(x) = Z^2 p(Z^{1/3}x)$ implies $E_{\mathrm{TF}}(Z) = -Z^{7/3} C_{\mathrm{TF}}$, where $C_{\mathrm{TF}} = -E_{\mathrm{TF}}(1)$. Theorem 5.21 of [3] uses a simple scaling argument to prove

$$R{:}K{:} -C_{\mathrm{TF}}{:}A = 1{:}3{:}3{:}7.$$

In their 1977 paper [4], Lieb and Simon proved that T-F theory describes the gross statistical properties of atoms and molecules in the large Z limit. For a nice discussion, see Section V of [3]. To describe their main theorem, we need some extra notation. The Hamiltonian for N electrons in an atom with nuclear carge Z is

$$H_{Z,N} = \sum_{k=1}^{N} \{-\Delta_k - Z\,|x_k|^{-1}\} + \sum_{i,j} |x_i - x_j|^{-i}.$$

Let $E_{Qn}(Z, N)$ denote the ground state energy of $H_{Z,N}$ (defined to be $\inf \operatorname{spec} H_{N,Z}$) taken over the Hilbert space $\Lambda_1^{N_{L^2}}(\mathbb{R}^3; C^q)$. This Hilbert space is the antisymmetric tensor product of q spin state wavefunctions. For electrons, $q=2$. However, it will be enough to do all our analysis with $q=1$. Let $\psi(x_1, ..., x_N; \sigma_1, ..., \sigma_q)$ be any normalized function in $\Lambda_1^N L^2(\mathbb{R}^3; C^q)$ and let

$$p_\psi(x) = N \sum_{i=1}^{q} \int |\psi(x, x_2, ..., x_N; \sigma_1, ..., \sigma_q)|^2 \, dx_2 \cdots dx_N.$$

Theorem 5.2 of [3] establishes the relationship between quantum mechanics and Thomas–Fermi theory. Let me describe it for the special case $q=1$.

THEOREM 5.2. OF [3]. *Let $\{\psi(x_1, ..., x_{N(Z)})\}$ be a sequence of normalized wavefunctions in $\Lambda_1^N L^2(\mathbb{R}^3)$ for which $|\langle \psi, H_{Z,N}\psi\rangle - E_{QM}| \, Z^{-7/3} = o(1)$ as $Z \to \infty$. Then,*

$$\left\langle \psi, \left(\sum_{k=1}^{N} -\Delta_{x_k} \right) \psi \right\rangle Z^{-7/3} \to K$$

$$\left\langle \psi, \left(\sum_{k=1}^{N} Z \, |x_k|^{-1} \right) \psi \right\rangle Z^{-7/3} \to V$$

$$\left\langle \psi, \left(\sum_{i<j} |x_i - x_j|^{-1} \right) \psi \right\rangle Z^{-7/3} \to R.$$

Moreover, if Ω is any bounded set in $\mathbb{R}^3$, then

$$Z^{-2} \int_\Omega p_\psi(Z^{-1/3}x) \, dx \to \int_\Omega p(x) \, dx.$$

In particular, this proves that $E(Z) \, Z^{-7/3}$ converges to $-C_{\mathrm{TF}}$ as $Z \to \infty$. Lieb and Simon were able to bound the error by $O(Z^{-1/30})$.

Notice that $-C_{\mathrm{TF}} Z^{7/3}$ is exactly the semiclassical phase space volume counting approximation to the ground state energy of

$$\sum_{k=1}^{N} \{ -\Delta_k - Zy(Z^{1/3} \, |x_k| \, \gamma^{-1}) \, |x_k|^{-1} \} - Z^{7/3} \, R. \tag{0.3}$$

This Hamiltonian provides a useful model in the sense that

$$-Zy(Z^{1/3}|x| \, \gamma^{-1})|x|^{-1} = -Z|x|^{-1} + \int p_Z(y)|x-y|^{-1} \, dy$$

correctly models the electrostatic potential that a given electron feels, *but* counts the interaction of each electron pair twice. Hence, subract the T-F repulsion. The semiclassical approximation gives

$$\frac{-q}{15\pi^2}\int (Zy(Z^{1/3}|x|\,\gamma^{-1})|x|^{-1})^{5/2}\,dx$$

as the ground state energy of the first term in (0.3). Because of the ratios of K, A, etc., the explicit value of γ, and the relationship between y and p, we know this is $-(2/3)\,C_{\mathrm{TF}}Z^{7/3}$. Since $Z^{7/3}R=(1/3)\,C_{\mathrm{TF}}Z^{7/3}$, the two terms add to give $-C_{\mathrm{TF}}Z^{2/3}$.

Recall that semiclassical phase space volume counting means decomposing $\mathbb{R}^3$ into little cubes $dx=dx_1\,dx_2\,dx_3$ and figuring out how many particles with total energy less than a given energy $-E$ can fit in each individual cube. If the potential energy is $-V(x)$ on dx, then each particle in dx must have kinetic energy $\leqslant (V(x)-E)_+$. The eigenvalues for the kinetic energy operator $-\Delta$ on a cube dx are

$$(2\pi)^2\,|dx|^{-2/3}\,(m_1^2+m_2^2+m_3^2),\qquad m_i\in\mathbb{Z}.$$

The number of eigenvalues with energy $\leqslant (V(x)-E)_+$ is approximately

$$\begin{aligned}N(E,x)&=\mathrm{Vol}\{(2\pi)^2\,|dx|^{-2/3}\,|\mathbf{m}|^2<(V(x)-E)_+\}\\&=(4/3)\,\pi(V(x)-E)_+^{3/2}\,\frac{|dx|}{(2\pi)^3}.\end{aligned}$$

For q spin states, exactly q particles can occupy each energy level. Hence, there are $q\cdot N(E,x)$ particles in dx with energy $\leqslant -E$. The total energy of all the electrons in dx is

$$-\int_0^\infty q\cdot N(E,x)\,dE=\frac{q}{15\pi^2}\int V(x)^{5/2}\,dx.$$

This calculation is asymptotically correct as the potential V gets large. In our case,

$$V(x)=Zy(Z^{1/3}|x|\,\gamma^{-1})|x|^{-1}.$$

In his 1952 paper [5], Scott argued that this semiclassical calculation does not accurately account for the innermost electrons—i.e., those with greatest negative energy. Since these electrons have energy $\sim Z^2$, there should be a correction to $-C_{\mathrm{TF}}Z^{7/3}$ of order Z^2. To uncover it, he replaced the semiclassical estimate for the sum of the energies of the first K electrons by its quantum mechanical analogue. Near the nucleus, $y(x)\sim 1$. Hence, he compared the semiclassical approximation for the sum of the first eigenvalue of $-\Delta_x - Z|x|^{-1}$ with the exact quantum calculation. The quantum mechanical quantity is larger by $Z^2(q/8 + O(K^{-1/2}))$. Scott took $q=2$ and $K \to \infty$. The $Z^2/4$ term is known as Scott's correction.

In Section I of this paper, we will prove that (0.3) is a lower bound for $H_{Z,N}$, modulo an error $\varepsilon(x)$ which has expectation $O(Z^{5/3})$ in the ground state. Calculation of the ground state for (0.3) reduces to one-dimensional eigenvalue problems. WKB theory provides a technique to sum eigenvalues of one-dimensional problems. We will see that application of the WKB method to (0.3) agrees with the semiclassical eigenvalue calculation of (0.3). Furthermore, we can explicitly estimate the errors from the WKB calculations. That is the subject of Section II. The different one-dimensional problems correspond to different spherical harmonics into which the eigenfunctions of the radial equation (0.3) decompose. For the smallest spherical harmonics, the WKB errors are so large as to make the analysis useless. For these l, we replace the one-dimensional Schrödinger operator

$$-\frac{d^2}{dx^2} - Zy(Z^{1/3}x)|x|^{-1} + l(l+1)\,x^{-2}$$

by the strictly smaller operator

$$-\frac{d^2}{dx^2} - Z|x|^{-1} + l(l+1)\,x^{-2}$$

and calculate explicitly. This has the same effect as Scott's replacement of semiclassical eigenvalue summing by quantum mechanics for the lowest energy levels. It proves

THEOREM. $E_{QM}(Z) \geqslant -C_{\mathrm{TF}} Z^{7/3} + (q/8)\,Z^2 + O(Z^{17/9}\log Z)$.

To simplify computations, we will prove the theorem for $q=1$. The proof for other q is an obvious generalization.

Subsequent to the completion of this paper, I learned that H. Siedentop [H. Siedentop, personal communication] established a similar upper bound to $E_{QM}(Z)$. Together, these two results prove Scott's famous conjecture.

I. Reduction to One-Dimensional Problems

In this section we derive a simple inequality that bounds the electron–electron interaction from below by the sum of the electrons' interaction with your favorite charge cloud. We will use the T-F density ρ_Z. As the discussion of Section 0 indicates, this is the correct choice as $Z \to \infty$.

For practical values of Z, other densities may lead to better results and optimization will probably be appropriate. Walter Thirring employed a similer lower bound to make numerical calculations. See [6].

To cast the inequality in its general setting, let $p(x) \geqslant 0$ be any $L'(\mathbb{R}^3)$ function for which all the quantities we write down are finite. Let $x_i \in \mathbb{R}^3$, $i = 1, ..., N$, be coordinates of the N electrons in our system. For $x \in \mathbb{R}^3$, let $R(x)$ be defined by

$$\int_{|x-y| \leqslant R(x)} p(y)\,dy = 1. \tag{I.1}$$

Let $d\mu_x$ be a normalized uniform surface measure on the sphere $|y-x| = R(x)$ about x. Our lower bound is derived from the following elementary potential theory inequality:

$$\frac{1}{2}\iint_{\mathbb{R}^3 \times \mathbb{R}^3} |x-y|^{-1} \left[\sum_{i=1}^{N} d\mu_{x_i}(x) - p(x)\,dx\right]\left[\sum_{j=1}^{N} d\mu_{x_j}(y) - p(y)\,dy\right] \geqslant 0.$$

Rearranging terms in (I.2) gives

$$\begin{aligned}\sum_{i<j} \iint |x-y|^{-1}\, d\mu_{x_i}(x)\, d\mu_{x_j}(y) &\\ \geqslant \sum_{i=1}^{N} \bigg\{ \iint |x-y|^{-1} p(y)\,dy\, d\mu_{x_i}(x) &\\ - \frac{1}{2}\iint |x-y|\, d\mu_{x_i}(x)\, d\mu_{x_i}(y) \bigg\} &\\ - \frac{1}{2}\iint |x-y|^{-1} p(x)\,p(y)\,dx\,dy. &\end{aligned}$$

The left side is clearly dominated by $\sum_{i<j} |x_i - x_j|^{-1}$. For each i, the bracketed term equals

$$\phi(x_i) = \int_{|y-x_i| > R(x_i)} |x_i - y|^{-1} p(y)\,dy + 1/2R(x_i). \tag{I.3}$$

We have obtained the desired lower bound

$$\sum_{i<j} |x_i - x_j|^{-1} \geqslant \sum_{i=1}^{N} \phi(x_1) - \frac{1}{2}\iint |x-y|^{-1} p(y)\,p(x)\,dx\,dy \tag{I.4}$$

and, hence, the operator inequality

$$H_{N,Z} \geqslant \sum_{k=1}^{N} \left\{ -\Delta_{x_k} - \frac{Z}{|x_k|} + \phi(x_k) \right\}$$
$$- \frac{1}{2} \iint |x-y|^{-1} p(y)\, p(x)\, dx\, dy. \tag{I.5}$$

Denote the $L_1^2(\mathbb{R}^3)$ operator $-\Delta_x - Z/|x| + \phi(x)$ by $\tilde{H}_Z$. The ground state energy of an atom of charge Z is given by

$$E(Z) = \inf_N \inf_{\|\psi\|_N = 1} \langle H_{Z,N}\psi, \psi \rangle.$$

Inequality (I.5) implies

$$E(Z) \geqslant \inf_N \inf_{\|\psi_N\| = 1} \sum_{i=1}^{N} \langle \tilde{H}_Z \psi, \psi \rangle - \frac{1}{2} \iint |x-y|^{-1} p(x)\, p(y)\, dx\, dy.$$

For given N, the second infinum is attained by $\psi(x_1, ..., x_N) = \psi_1(x_1) \wedge \cdots \wedge \psi_N(x_N)$, where ψ_i is the eigenfunction corresponding to the ith lowest eigenvalue E_i of $\tilde{H}_Z$ acting on $L_1^2(\mathbb{R}^3)$. Let $-E_0^Z < -E_1^Z < \cdots < 0$ be the negative eigenvalues of $H_{Z,x}$. We have shown

$$E(Z) \geqslant \sum_{k=0}^{\infty} (-E_k^Z) - \frac{1}{2} \iint |x-y|\, p(x)\, p(y)\, dx\, dy. \tag{I.6}$$

This is a big step. It reduces the calculation of $E(Z)$ to a one electron eigenvalue problem. Now assume $\rho(x)$ is a radial function of $x \in \mathbb{R}^3$. This trivially implies that $\phi(x)$ is also radial. The eigenfunctions $\psi(x)$ of $\tilde{H}_Z$ decompose as products of radial functions and spherical harmonics. For angular momentum $l(l+1)$, the radial function f is (after the usual change of variable) an eigenfunction for

$$-\frac{d^2}{dr^2} f + \{ -Z/r + \phi(r) + l(l+1)/r^2 \} f = -Ef. \tag{I.7}$$

Let $-E_0^{Z,l} < -E_1^{Z,l} < \cdots < 0$ be the negative eigenvalues for (I.7). This reduces (I.6.) to

$$E(Z) \geqslant \sum_{l=0}^{\infty} (2l+1) \cdot \sum_{k=0}^{\infty} (-E_K^{Z,l})$$
$$- \frac{1}{2} \iint |x-y|^{-1} p(x)\, p(y)\, dx\, dy. \tag{I.8}$$

Once we have our hands on $\phi(r)$, a tedious and taxing application of the WKB approximation gives a good lower bound. To prove Scott's conjecture, let $p(x)$ be the Thomas–Fermi density $p_Z(x)$ for a charge Z neutral atom. It is much more convenient to deal with

$$\tilde{\phi}(x) = \iint |x-y|^{-1} p_Z(y)\, dy$$

than with the $\phi(x)$ defined by (I.3). The two differ by the error

$$\varepsilon(x) = \phi(x) - \tilde{\phi}(x) = 1/2R(x, Z) - \int_{|x-y| < R(x, Z)} |x-y|^{-1} p_Z(y)\, dy. \tag{I.9}$$

The following lemma allows us to replace ϕ by $\tilde{\phi}$.

LEMMA. *Let $\psi_Z(x_1, ..., x_N)$ be the ground state wavefunction*[1] *for an atom of charge Z. Then, $\langle (\sum_{i=1}^{N} \varepsilon(x_i))\, \psi, \psi \rangle = O(Z^{5/3})$ as $Z \to \infty$.*

Proof. Define

$$\tilde{p}_Z(x) = N \int_{x_2 \cdots x_N} \cdots \int |\psi(x, x_2, ..., x_N)|^2\, dx_2 \cdots dx_N.$$

As we saw in the introduction, Theorem 5.2 of [3] states that $Z^{-2}\tilde{p}_Z(xZ^{-1/3}) \to \rho_1(x)$ in the various senses, as $Z \to \infty$, where p_1 is the $Z=1$ T-F density. By antisymmetry,

$$\left\langle \left(\sum_{i=1}^{N} \varepsilon(x_1) \right) \psi, \psi \right\rangle = \int_{\mathbb{R}^3} \varepsilon(x)\, \tilde{p}_Z(x)\, dx.$$

By definition of $R(x)$, $\varepsilon(x)$ is strictly negative and bounded in absolute value by

$$\int_{|x-y| < R(x, Z)} |x-y|^{-1} p_Z(y)\, dy.$$

Hence, we must estimate

$$\iint_{|x-y| < R(x, Z)} |x-y|^{-1} p_Z(y)\, \tilde{p}_Z(x)\, dx\, dy.$$

[1] If $E(Z)$ is degenerate, ψ_Z can be any ground state wavefunction as far as Lemma 1 is concerned. If $E(Z)$ is not an eigenvalue, but merely $\inf_N \inf \operatorname{spec} H_{Z,N}$, then it is possible to define an approximating sequence ψ_Z in such a way that the lemma still holds. See [3, p. 623].

Change variables $y=\bar{y}Z^{-1/3}$, $x=\bar{x}Z^{-1/3}$. The integral becomes

$$Z^{7/3}\iint_{|x-y|<Z^{1/3}R(Z^{-1/3}x,\,Z)} |x-y|^{-1}Z^{-2}$$
$$\times\, \tilde{p}_Z(xZ^{-1/3})\,Z^{-2}p_Z(yZ^{-1/3})\,dx\,dy$$
$$=Z^{5/3}\int_{x\in\mathbb{R}^3} Z^{-2}\tilde{p}_Z(xZ^{-1/3})\,Z^{2/3}$$
$$\times\left[\int_{|x-y|<Z^{1/3}R(Z^{-1/3}x,\,Z)} |x-y|^{-1}p_1(y)\,dy\,dx\right].$$

Define $\tilde{R}(x,Z)=Z^{1/3}R(Z^{-1/3}x,Z)$ and

$$\phi(x,Z)=Z^{2/3}\int_{|x-y|<\tilde{R}(x,Z)} |x-y|^{-1}p_1(y)\,dy.$$

Notice that the definition of $R(x,Z)$ implies that $\tilde{R}(x,Z)$ is defined by:

$$\iint_{|x-y|<\tilde{R}(x,Z)} p_1(y)\,dy=Z^{-1}.$$

As $Z\to\infty$,

$$\tilde{R}(x,Z)\to \text{const.}\,(p_1(x)\,Z)^{-1/3}$$
$$\phi(x,Z)\to \text{const.}\,p_1(x)^{1/3}.$$

This convergence is uniform for $|x|>\varepsilon$. As $x\to\infty$, $p_1(x)\approx\text{const.}\,x^{-6}$. As $x\to 0$, $p_1(x)=\text{const.}\,X^{-3/2}(1+O(x))$. In the regimes $x\to\infty$ and $Z^{-2/3}<|x|<\varepsilon$, $p_1(x)$ changes by at most a factor over the ball about x for which p integrates to z^{-1}. Hence,

$$\phi(x,Z)<\text{const.}\,p_1(x)^{1/3}$$

in these cases. By uniform convergence, it also holds when $|x|$ is $>\varepsilon$ but not yet in the large $|x|$ asymptotic regime. Furthermore,

$$\phi(x,Z)<\phi(0,Z)<Z^{1/3}$$

for all Z. In particular, it holds when $|x|<Z^{-2/3}$. This implies

$$\phi(x,Z)<\text{const.}\,p_1(x)^{1/3}\qquad\text{for all } x,$$

independently of Z.

The well-known Lieb–Thirring stability of matter inequality (see [6, p. 11]) states

$$\langle \psi, \Delta_N \psi \rangle \geqslant \text{const.} \int \tilde{p}_Z^{5/3}(x)\, dx.$$

After rescaling, it gives

$$\langle \psi, \Delta_N \psi \rangle Z^{-7/3} \geqslant \text{const.} \int (Z^{-2} \tilde{p}_Z(xZ^{-1/3}))^{5/3}\, dx.$$

By Theorem 5.2 of [3] the left-hand side converges to the constant K. Holder's inequality implies

$$\int_{x \in \mathbb{R}^3} z^{-2} \tilde{p}_Z(xZ^{-1/3})\, \phi(x, Z)\, dx$$
$$\leqslant \left(\int (Z^{-2} \tilde{p}_Z(xZ^{-1/3}))^{5/3}\, dx \right)^{3/5} \left(\int \phi(x, Z)^{5/2}\, dx \right)^{2/5}.$$

The first factor converges to $K^{3/5}$. The second is

$$\leqslant \text{const.} \left(\int p_1(x)^{5/6} \right)^{2/5} < \infty. \quad \blacksquare$$

Staying with the notation of Section 0, let us write the screened potential

$$\left\{ -Z\, |x|^{-1} + \int |x-y|^{-1} \rho(y)\, dy \right\} = Zy(Z^{1/3} \gamma^{-1} |x|)\, |x|^{-1}.$$

We must compute a lower bound for the sum of the negative eigenvalues $-E_0^{Z,l} < -E_1^{Z,l} < \cdots < 0$ of

$$\frac{-d^2}{dr^2} w + \{ -Zy(Z^{1/3} \gamma^{-1} r)\, r^{-1} + l(l+1)\, r^{-2} \}\, w = -Ew. \tag{I.10}$$

Let $L(Z)$ be the largest integer less than $Z^{1/9}$. Since $y \leqslant 1$, the eigenvalues of the hydrogenic atom

$$-\frac{d^2}{dr^2} w + \{ -Zr^{-1} + l(l+1)\, r^{-2} \}\, w = -Ew$$

are strictly less than those of (I.10). Furthermore, they give a useful lower bound when $l \leqslant L(Z)$. We can calculate it:

$$\sum_{l=0}^{L(Z)} (2l+1) \left(\sum_{k=0} -E_k^{Z,l} \right) \geqslant \sum_{l=0}^{L(Z)} (2l+1) \sum_{k=1}^{\infty} Z^2/4(k+l)^2.$$

By approximating each sum on k by the corresponding integral and estimating the error, it is easy to calculate

$$\sum_{l=0}^{L} (2l+1) \sum_{k=1}^{\infty} (l+k)^{-2} = 2(L+1) - \frac{1}{2} + O(L^{-1}).$$

This implies

$$\sum_{l=0}^{L(Z)} (2l+1) \sum_{k=0} -E_k^{Z,l} \geqslant -Z^2 \left(\frac{L(Z)+1}{2} - 1/8 + O(L(Z)^{-1}) \right). \qquad \text{(I.11)}$$

For $l \geqslant L(Z)+1$, the WKB approximation helps us sum the eigenvalues of (I.10). After rescaling, (I.10) becomes

$$\frac{d^2}{dr^2} w + Z^{2/3} \{ y(\gamma^{-1} r)\, r^{-1} - \Omega r^{-2} - \mathscr{E} \}\, w = 0, \qquad \text{(I.12)}$$

where $\Omega = l(l+1)\, Z^{-2/3}$, $\mathscr{E} = EZ^{-4/3}$. Since $y(r) \sim 1$ as $r \to 0$, there is exactly one linearly independent solution of (I.12) which is L^2 as $r \to 0$. We must find the "eigenvalue" $\mathscr{E}_k = E_k^{Z,l} Z^{-4/3}$ for which this solution decays exponentially at infinity. WKB theory gives the large Z asymptotic answer

$$(Z^{1/3}\pi) \int \{ y(\gamma^{-1} r)\, r^{-1} - \Omega r^{-2} - \mathscr{E}_k \}_+^{1/2} dr = k + 1/2. \qquad \text{(I.13)}$$

The main work in this article goes into proving

WKB THEOREM. *Assume* $\Omega > L(Z)(L(Z)+1)\, Z^{-2/3}$. *Let* $-\mathscr{E}(\Omega) = \min_x \{ \Omega x^{-2} - y(\gamma^{-1} x)\, x^{-1} \}$ *and assume* Ω *is small enough that* $\mathscr{E}(\Omega) > 0$. *Let* $\mathscr{E}_k$ *with* $-\mathscr{E}(\Omega) < -\mathscr{E}_0 < -\mathscr{E}_1 < \cdots < 0$ *be the negative eigenvalue of* (I.12) *and define* $\delta(Z, \Omega, \mathscr{E}_k)$ *by*

$$(Z^{1/3}/\pi) \int \{ y(\gamma^{-1} x)\, x^{-1} - \Omega x^{-2} - \mathscr{E}_k \}_+^{1/2} dx = k + 1/2 + \delta(Z, \Omega, \mathscr{E}_k). \qquad \text{(I.14)}$$

There is a constant M *so that if*

$$-\mathscr{E}(\Omega) \leqslant -\mathscr{E}_k \leqslant -\mathscr{E}(\Omega) + 10 M Z^{-1/3} \Omega^{-1/3}$$

then $|\delta(Z, \Omega, \mathscr{E}_k)| = o(1)$ *uniformly in* Ω *as* $Z \to \infty$, *and if*

$$-\mathscr{E}(\Omega) + 10 M Z^{-1/3} \Omega^{-3/2} \leqslant -\mathscr{E}_k \leqslant 0$$

then $|\delta(Z, \Omega, \mathscr{E}_k)| \leqslant M Z^{-1/3} \Omega^{-3/2} (\mathscr{E}(\Omega) - \mathscr{E}_k)^{-1}$.

Notice that $\{ \Omega x^{-2} - y(\gamma^{-1} x)\, x^{-1} \} > \{ \Omega x^{-2} - x^{-1} \} > -(4\Omega)^{-1}$.

Hence, $\mathscr{E}(\Omega) < (4\Omega)^{-1}$. Furthermore, since $y(x) \approx 144x^{-3}$ as $x \to \infty$, $\{\Omega x^{-2} - y(\gamma^{-1}x)\, x^{-1}\}$ is positive for large x. As Ω increases, the region on which this potential is negative shrinks monotonically. At some sufficiently large $\Omega = \bar{\Omega}$, $\mathscr{E}(\bar{\Omega}) = 0$. For $\Omega > \bar{\Omega}$, (I.12) has no negative eigenvalues. For $\Omega < \bar{\Omega}$, they range between $-\mathscr{E}(\Omega)$ and 0. The *WKB Theorem* describes precisely the extent to which (I.13) gives an approximation to these eigenvalues.

We prove the WKB Theorem in Section II. In the remainder of this section we show how the WKB Theorem implies the theorem of this paper.

Define

$$G(\Omega, \mathscr{E}) = (1/\pi) \int \{y(x)\, x^{-1} - \Omega x^{-2} - \mathscr{E}\}_+^{1/2}\, dx.$$

For $\Omega = l(l+1)\, Z^{-2/3}$,

$$\sum_{k=0} E_k^{Z,l} = Z^{4/3} \sum_{k=0} \mathscr{E}_k.$$

We must estimate $\sum_{k=0} \mathscr{E}_k$. If $-\mathscr{E}_k$ is the smallest negative eigenvalue, assume $\mathscr{E}_{K+1} = 0$. We can rewrite

$$\sum_{k=0} \mathscr{E}_k = \sum_{k=0}^{K} (k+1)(\mathscr{E}_k - \mathscr{E}_{k+1}).$$

In Section II, we will calculate the first two derivatives of $G(\Omega, \mathscr{E})$ with respect to $\mathscr{E}$. For now, simply note that they exist. For $k < K$, where $\mathscr{E}_K$ is the smallest of the $\mathscr{E}_k$, this implies

$$\begin{aligned} Z^{1/3} \int_{\mathscr{E}_{k+1}}^{\mathscr{E}_k} G(\Omega, \mathscr{E})\, d\mathscr{E} \geqslant (1/2) Z^{1/3} \Bigg\{ &\int_{\mathscr{E}_{k+1}}^{\mathscr{E}_k} \left[G(\Omega, \mathscr{E}_k) + \frac{d}{d\mathscr{E}} G(\Omega, \mathscr{E}_k)(\mathscr{E} - \mathscr{E}_k) \right. \\ &\left. + (1/2) \frac{d^2}{d\mathscr{E}^2} G(\Omega, \bar{\mathscr{E}}_k)(\mathscr{E} - \mathscr{E}_k)^2 \right] \\ &+ \int_{\mathscr{E}_{k+1}}^{\mathscr{E}_k} \left[G(\Omega, \mathscr{E}_{k+1}) + \frac{d}{d\mathscr{E}} G(\Omega, \mathscr{E}_{k+1})(\mathscr{E} - \mathscr{E}_{k+1}) \right. \\ &\left. + (1/2) \frac{d^2}{d\mathscr{E}^2} G(\Omega, \bar{\mathscr{E}}_k)(\mathscr{E} - \mathscr{E}_{k+1})^2 \right] \Bigg\} \end{aligned}$$

for some $\bar{\mathscr{E}}_k \in [\mathscr{E}_k, \mathscr{E}_{k+1}]$. By (I.14), this is

$$\begin{aligned} &\geqslant (k+1)(\mathscr{E}_k - \mathscr{E}_{k+1}) \\ &\quad + (1/2)[\delta(Z, \Omega, \mathscr{E}_{k+1}) + \delta(Z, \Omega, \mathscr{E}_k)](\mathscr{E}_k - \mathscr{E}_{k+1}) \\ &\quad - Z^{1/2} \left| \frac{d^2}{d\mathscr{E}^2} G(\Omega, \bar{\mathscr{E}}_k) \right| (\mathscr{E}_k - \mathscr{E}_{k+1})^3. \end{aligned}$$

Notice that once Z is large enough the *WKB Theorem* implies $|\delta(Z, \Omega, \mathscr{E}_k)| < 1/10$, independently of Ω and $\mathscr{E}_k$. Hence (I.14) and the mean value theorem imply

$$|\mathscr{E}_k - \mathscr{E}_{k+1}| < 2Z^{-1/3} \left| \frac{d}{d\mathscr{E}} G(\Omega, \bar{\bar{\mathscr{E}}}_k) \right|^{-1} \tag{I.15}$$

for some $\bar{\bar{\mathscr{E}}}_k \in [\mathscr{E}_{k+1}, \mathscr{E}_k]$. For $k < K$ this implies

$$\begin{aligned} Z^{1/3} \int_{\mathscr{E}_{k+1}}^{\mathscr{E}_k} G(\Omega, \mathscr{E})\, d\mathscr{E} &\geqslant (k+1)(\mathscr{E}_k - \mathscr{E}_{k+1}) \\ &- \Bigg\{ |\delta(Z, \Omega, \mathscr{E}_k)| + |\delta(Z, \Omega, \mathscr{E}_{k+1})| \\ &+ 4Z^{-1/3} \left| \frac{d^2}{d\mathscr{E}^2} G(\Omega, \mathscr{E}) \right| \left| \frac{d}{d\mathscr{E}} G(\Omega, \mathscr{E}) \right|^{-2} \Bigg\} \cdot (\mathscr{E}_k - \mathscr{E}_{k+1}). \end{aligned}$$

Also,

$$\begin{aligned} (K+1)(\mathscr{E}_K - \mathscr{E}_{K+1}) &= (K+1)\, \mathscr{E}_K \\ &= Z^{1/3} \int_0^{\mathscr{E}_k} G(\Omega, \mathscr{E}_K) + (1/2 - \delta(Z, \Omega, \mathscr{E}_K))\, \mathscr{E}_K. \end{aligned}$$

Since G is decreasing with increasing $\mathscr{E}$ this is

$$\leqslant Z^{1/3} \int_0^{\mathscr{E}_k} G(\Omega, \mathscr{E})\, d\mathscr{E} + (1/2 - \delta(Z, \Omega, \mathscr{E}_K)) \cdot \mathscr{E}_K. \tag{I.16}$$

Inequality (I.15) implies

$$\mathscr{E}_K < 2Z^{-1/3} \left| \frac{d}{d\mathscr{E}} G(\Omega, \bar{\bar{\mathscr{E}}}_K) \right|^{-1}.$$

Since $|\delta|$ is small compared to 1,

$$|(1/2 - \delta(Z, \Omega, \mathscr{E}_K)) \cdot \mathscr{E}_K| < 2Z^{-1/3} \left| \frac{d}{d\mathscr{E}} G(\Omega, \bar{\bar{\mathscr{E}}}_K) \right|^{-1}.$$

Hence,

$$Z^{1/3} \int_0^{\mathscr{E}_K} G(\Omega, \mathscr{E})\, d\mathscr{E} \geqslant (K+1)\, \mathscr{E}_K - 2Z^{-1/3} \left| \frac{d}{d\mathscr{E}} G(\Omega, \bar{\bar{\mathscr{E}}}_K) \right|^{-1}. \tag{I.16$'$}$$

To apply (I.16) and (I.16′) we use the following estimates, proved in Section II. Assume $\Omega > L(Z)(L(Z)+1)\, Z^{-2/3}$.

Estimate 1.

$$\left|\frac{d}{d\mathscr{E}} G(\Omega, \mathscr{E})\right| \geqslant M^{-1}\mathscr{E}_k^{-3/2} \qquad \text{if} \quad \mathscr{E}_k > 10$$

$$\left|\frac{d}{d\mathscr{E}} G(\Omega, \mathscr{E})\right| \geqslant M^{-1} \qquad \text{if} \quad \mathscr{E}_k < 10.$$

Estimate 2. If $-\mathscr{E}_k > -\mathscr{E}(\Omega) + 10MZ^{-1/3}\Omega^{-3/2}$ then

$$\left|\frac{d^2}{d\mathscr{E}^2} G(\Omega, \bar{\bar{\mathscr{E}}}_k)\right| \left|\frac{d}{d\mathscr{E}} G(\Omega, \bar{\bar{\mathscr{E}}}_k)\right|^{-2} \leqslant MZ^{-1/3}\Omega^{-3/2} \cdot (\mathscr{E}(\Omega) - \mathscr{E}_k)^{-1}.$$

Estimate 3. Let $K(Z, \Omega) = \min\{k \mid -\mathscr{E}_k > -\mathscr{E}(\Omega) + 10MZ^{-1/3}\Omega^{-3/2}\}$. Then for sufficiently large Z, $K(Z, \Omega)$ is uniformly bounded, independently of Z and Ω.

Estimate 1 and (I.16′) imply

$$(K+1)\,\mathscr{E}_K \leqslant Z^{1/3} \int_0^{\mathscr{E}_K} G(\Omega, \mathscr{E})\, d\mathscr{E} + MZ^{-1/3}. \tag{I.17}$$

Estimate 2, (I.16), and the WKB Theorem imply

$$\sum_{k=K(Z,\Omega)}^{K-1} (k+1)(\mathscr{E}_k - \mathscr{E}_{k+1}) \leqslant Z^{1/3} \int_{\mathscr{E}_{K(Z,\Omega)}}^{\mathscr{E}_K} G(\Omega, \mathscr{E})\, d\mathscr{E}$$
$$+ 5MZ^{-1/3}\Omega^{-3/2} \sum_{k=K(Z,\Omega)}^{K-1} (\mathscr{E}(\Omega) - \mathscr{E}_k)^{-1} \cdot (\mathscr{E}_k - \mathscr{E}_{k+1}).$$

Estimate 3 implies

$$\sum_{k=0}^{K(Z,\Omega)-1} (k+1)(\mathscr{E}_k - \mathscr{E}_{k+1}) \leqslant (\text{large const.})\, Z^{-1/3}\Omega^{-3/2}.$$

Perhaps sacrificing a factor which is very close to 1, we can replace

$$\sum_{k=K(Z,\Omega)}^{K-1} (\mathscr{E}(\Omega) - \mathscr{E}_k)^{-1}\, (\mathscr{E}_k - \mathscr{E}_{k+1})$$

by the corresponding integral. To see this, notice that (I.15), Estimate 1, and the fact that $\mathscr{E}(\Omega) \leqslant (4\Omega)^{-1}$ imply that the eigenvalue gap $|\mathscr{E}_k - \mathscr{E}_{k+1}|$ is small compared to $|\mathscr{E}(\Omega) - \mathscr{E}_k|$ as long as $k \geqslant K(Z, \Omega)$. After a change of variables, the integral equals

$$\int_{10MZ^{-1/3}\Omega^{-3/2}}^{\mathscr{E}(\Omega)} \mathscr{E}^{-1} d\mathscr{E},$$

which is

$$\leqslant \int_{10MZ^{-1/3}\Omega^{-3/2}}^{(4\Omega)^{-1}} \mathscr{E}^{-1} d\mathscr{E} \leqslant \log Z^{1/3}\Omega + \text{const.}$$

Put all this together and we find that for $\Omega \in [L(Z)(L(Z)+1)\, Z^{-2/3}, \bar{\Omega}]$ and Z sufficiently large,

$$\sum_{k=0}^{K} \mathscr{E}_k \leqslant Z^{1/3} \int_0^{\mathscr{E}(\Omega)} G(\Omega, \mathscr{E})\, d\mathscr{E} + (\text{large const.})\, Z^{-1/3}\Omega^{-3/2} \log Z^{1/3}. \tag{I.18}$$

Recalling that $\Omega = l(l+1)\, Z^{-2/3}$, this implies

$$\sum_{l=L(Z)+1} (2l+1) \left(\sum_{k=0} -E_k^{Z,l} \right) \geqslant -Z^{7/3} \sum_{l=L(Z)+1} (2l+1)\, Z^{-2/3} \int_{\mathscr{E}>0} G(l(l+1)\, Z^{-2/3}, \mathscr{E})\, d\mathscr{E} - Z^2 \text{ const. } L(Z)^{-1} \log Z^{1/3}. \tag{I.19}$$

To calculate the sum on the right side of (I.19), let

$$\mathscr{G}(\Omega) = \int_{\mathscr{E}>0} G(\Omega, \mathscr{E})\, d\mathscr{E} = \left(\frac{2}{3\pi}\right) \int_{R^3} [y(x)\, x^{-1} - \Omega x^{-2}]_+^{3/2}\, dx.$$

Notice that $\mathscr{G}(\Omega)$ is a convex function of Ω which decreases for $\Omega < \bar{\Omega}$ and is zero for $\Omega \geqslant \bar{\Omega}$. We compare the sum in (I.19) to the corresponding integral over Ω. Let $\bar{L}(Z) = \max\{l \mid l(l+1)\, Z^{-2/3} < \bar{\Omega}\}$.

$$\begin{aligned}
&\sum_{l=L(Z)+1}^{\bar{L}(Z)} (2l+1)\, Z^{-2/3}\, \mathscr{G}(l(l+1)\, Z^{-2/3}) \\
&\quad = \int_{\lambda > L(Z)+1} (2\lambda+1)\, Z^{-2/3}\, \mathscr{G}(\lambda(\lambda+1)\, Z^{-2/3})\, d\lambda \\
&\qquad + Z^{-2/3} \sum_{l=L(Z)+1} \int_l^{l+1} \{(2l+1)\, \mathscr{G}(l(l+1)\, Z^{-2/3}) \\
&\qquad - (2\lambda+1)\, \mathscr{G}(\lambda(\lambda+1)\, Z^{-2/3})\}\, d\lambda \\
&\quad = \int_{\Omega > (L(Z)+1)(L(Z)+2)\, Z^{-2/3}} G(\Omega)\, d\Omega + Z^{-2/3} \sum_{l=L(Z)+1} \int_l^{l+1} \{\ \}\, d\lambda.
\end{aligned} \tag{I.20}$$

Since $\mathscr{G}$ is convex,

$$-\mathscr{G}(\lambda(\lambda+1)\,Z^{-2/3}) < -\mathscr{G}(l(l+1)\,Z^{-2/3}) \\ + (l(l+1)-\lambda(\lambda+1))\,Z^{-2/3}\,\mathscr{G}'(l(l+1)\,Z^{-2/3}).$$

Hence, the bracketted expression in (I.20) satisfies

$$\{\ \} < ((2l+1)-(2\lambda+1))\,\mathscr{G}(l(l+1)\,Z^{-2/3}) \\ + (2\lambda+1)(l(l+1)-\lambda(\lambda+1))\,Z^{-2/3}\,\mathscr{G}'(l(l+1)\,Z^{-2/3}).$$

Upon integration,

$$\int_{\lambda=l}^{l+1} \{\ \}\,d\lambda < -\mathscr{G}(l(l+1)\,Z^{-2/3}) \\ - 2(l+1)^2\,Z^{-2/3}\,\mathscr{G}'(l(l+1)\,Z^{-2/3}).$$

Since $\mathscr{G}$ is convex and $\mathscr{G}(\Omega)=0$ for large Ω,

$$\mathscr{G}(l(l+1)\,Z^{-2/3} > \sum_{k=l+1} -2kZ^{-2/3}\,\mathscr{G}'(k(k+1)\,Z^{-2/3}).$$

Hence,

$$\begin{aligned} &\sum_{l=L(Z)+1} -\mathscr{G}(l(l+1)\,Z^{-2/3}) \\ &\quad\leqslant \sum_{l=L(Z)+1}\ \sum_{k=l+1} 2k\,Z^{-2/3}\,\mathscr{G}'(k(k+1)\,Z^{-2/3}) \\ &\quad= \sum_{k=L(Z)+2} \left[\sum_{l=L(Z)+1}^{k-1} 1\right] 2k\,Z^{-2/3}\,\mathscr{G}'(k(k+1)\,Z^{-2/3}) \\ &\quad= \sum_{k=L(Z)+2} 2k(k-L(Z)-1)\,Z^{-2/3}\,\mathscr{G}'(k(k+1)\,Z^{-2/3}). \end{aligned}$$

Consequently,

$$\begin{aligned} &\sum_{l=L(Z)+1} \int_{\lambda=l}^{l+1} \{\ \}\,d\lambda \\ &\quad< \sum_{l=L(Z)+2}^{\bar{L}(Z)} 2l(l-L(Z)-1)\,Z^{-2/3}\mathscr{G}'(l(l+1)\,Z^{-2/3}) \\ &\qquad- \sum_{l=L(Z)+1}^{\bar{L}(Z)} 2(l+1)^2\,Z^{-2/3}\mathscr{G}'(l(l+1)\,Z^{-2/3}) \end{aligned}$$

$$= \sum_{l=L(Z)+2}^{\infty} -2l\left(3+L(Z)+\frac{2}{l}\right) Z^{-2/3}\mathscr{G}'(l(l+1)\,Z^{-2/3})$$
$$-2(L(Z)+2)^2 Z^{-2/3}\mathscr{G}'(L(Z)(L(Z)+1)\,Z^{-2/3})$$
$$<(L(Z)+3+O(L(Z)^{-1}))\,\mathscr{G}(L(Z)(L(Z)+1)\,Z^{-2/3})$$
$$-2(L(Z)+2)^2 Z^{-2/3}\mathscr{G}'(L(Z)(L(Z)+1)\,Z^{-2/3}). \qquad \text{(I.21)}$$

Since $y(x)=1+o(x)$ as $x\to 0$, the asymptotics of $\mathscr{G}(\Omega)$ as $\Omega\to 0$ can be computed in terms of the Beta function,

$$\begin{aligned}
\mathscr{G}(\Omega) &= \frac{2}{3\pi}\int [y(r)/r-\Omega/r^2]_+^{3/2}\,dr \\
&= \frac{2}{3\pi}\int [ry(r)-\Omega]_+^{3/2}\,r^{-3}dr \\
&= \frac{2}{3\pi}\int_0^{\varepsilon} [ry(r)-\Omega]_+^{3/2}\,r^{-3}dr \\
&\quad + \frac{2}{3\pi}\int_{\varepsilon}^{\infty} [ry(r)-\Omega]_+^{3/2}\,r^{-3}dr.
\end{aligned}$$

As $\Omega\to 0$, the second term is $O(1)$. Also, the first term is within $O(1)$ of

$$\begin{aligned}
&\frac{2}{3\pi}\int_0 [r-\Omega]_+^{3/2}\,r^{-3}dr \\
&= \Omega^{-1/2}\frac{2}{3\pi}\int_1^{\varepsilon/\Omega} [r-1]^{3/2}\,r^{-3}dr \\
&= \Omega^{-1/2}\frac{2}{3\pi}\int_1^{\infty} [r-1]^{3/2}\,r^{-3}dr + O(1) \qquad \text{as} \quad \Omega\to 0 \\
&= \Omega^{-1/2}\frac{2}{3\pi}\frac{\Gamma(5/2)\,\Gamma(1/2)}{\Gamma(3)} + O(1) \\
&= \frac{\Omega^{-1/2}}{4} + O(1).
\end{aligned}$$

A similar calculation shows that

$$\mathscr{G}'(\Omega) = -\tfrac{1}{8}\Omega^{-3/2} + O(\Omega^{-1/2}) \qquad \text{as} \quad \Omega\to 0.$$

Combining this with (I.19), (I.20), (I.21), we obtain

$$\sum_{l=L(Z)+1} (2l+1)\left(\sum_{k=0} -E_k^{Z,l}\right)$$

$$\geqslant -Z^{7/3}\int_{\Omega>(L(Z)+1)(L(Z)+2)Z^{-2/3}} \mathscr{G}(\Omega)\,d\Omega$$

$$-(Z^{2/4})-Z^2 \text{ const. } L(Z)^{-1}\log Z^{1/3}. \tag{I.22}$$

Since $\mathscr{G}(\Omega)=\Omega^{-1/2}/4+O(1)$ as $\Omega\to 0$ and $L(Z)\approx Z^{1/9}$,

$$Z^{7/3}\int_{\Omega<(L(Z)+1)(L(Z)+2)Z^{-1/3}} \mathscr{G}(\Omega)\,d\Omega$$

$$=\frac{1}{2}\left(L(Z)+1+\frac{1}{2}\right)Z^2+O(Z^2L(Z)^{-1}+Z^{5/3}L(Z)^2).$$

Inequality (I.22) then implies

$$\sum_{l=L(Z)+1}^{\infty} (2l+1)\sum_{k=0}^{\infty} (E_k^{Z,l})$$

$$\geqslant Z^{7/3}\int G(\Omega)\,d\Omega+(L(Z)+1)\,Z^2/2+O(Z^{17/9}\log Z). \tag{I.23}$$

Notice that

$$\int_{\Omega=0}^{\infty}\mathscr{G}(\Omega)\,d\Omega=(2/3\pi)\int_0^{\infty}\int_0^{\infty}\{y(r\gamma^{-1})\,r^{-1}-\Omega r^{-2}\}_+^{3/2}\,dr\,d\Omega$$

$$=(15\pi^2)^{-1}\int_{\mathbb{R}^3}(y(x\gamma^{-1})|x|^{-1})^{5/2}\,dx.$$

As we pointed out in Section 0, this equals $(2/3)\,C_{\mathrm{TF}}$. Combine (I.23) with (I.11) to obtain

$$\sum_{l=0}(2l+1)\left(\sum_{k=0} -E_k^{Z,l}\right)$$

$$\geqslant -(2/3)\,C_{\mathrm{TF}}Z^{7/3}+\frac{1}{8}Z^2+O(Z^{17/9}\log Z^{1/3}). \tag{I.24}$$

Recall from Section 0

$$\frac{1}{2}\iint |x-y|^{-1}\,\rho(x)\,\rho(y)\,dx\,dy=(1/3)\,C_{\mathrm{TF}}.$$

Inequalities (I.8) and (I.24) prove

$$E(Z) \geqslant -C_{\mathrm{TF}} Z^{7/3} + \tfrac{1}{8} Z^2 + O(Z^{17/9} \log Z^{1/3}).$$

In the next sections we will prove the WKB Theorem and Estimates 1, 2, and 3.

II. WKB METHOD FOR $[\Omega/x^2 - y(x)/x]$

The WKB eigenvalue equation (I.14) is derived by approximating solutions w to (I.12) in various ways on various intervals of the positive real axis and matching boundary conditions. The particular approximation used on a given region of the x-axis depends on the size of the potential

$$p(x) = [\Omega/x^2 - y(x)/x + \mathscr{E}].$$

(For convenience, forget about γ^{-1}.)

The errors involved in this approximation can be bounded in terms of p and its derivatives. As such it is essential to understand how p behaves.

Let $\mathscr{E} = 0$. We know what happens to $p(x)$ when we take other $\mathscr{E}$. Assume $\Omega < \bar{\Omega}$, where

$$\min_x \{\bar{\Omega}/x^2 - y(x)/x\} = 0.$$

This means $p(x) < 0$ for some interval of the x-axis. Define

$$\mathscr{E}(\Omega) = -\min_x \{\Omega/x^2 - y(x)/x\}.$$

Several properties of $p(x)$ are immediately evident from the asymptotic properties of $y(x)$ quoted in Section 0. Since $1 - wx \leqslant y(x) < 1$,

$$\Omega/x^2 - 1/x < p(x) < \Omega/x^2 - 1/x + w.$$

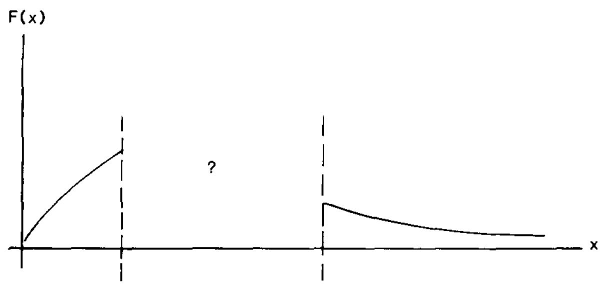
This is useful when $x \to 0$. It shows, in particular, that $\mathscr{E}(\Omega) > -\min\{\Omega/x^2 - 1/x\} = (4\Omega)^{-1}$. Let $\bar{x}$ be so large that for $x > \bar{x}$, $y(x)$ and its first three derivatives equal $144x^{-3}$ and its first three derivatives within a factor $1 \pm 1/10$. Since $\Omega/x^2 \gg 144x^4$ for large x, with both quantities dying rapidly, this implies the existence of two critical points—one where $p(x)$ attains its minimum $-\mathscr{E}(\Omega)$, and one where $p(x)$ attains a positive local maximum before it decreases to zero at infinity. To apply WKB theory, we need to know that these are the only critical points.

The condition for x to be a critical is

$$p'(x) = -2\Omega/x^3 + y(x)/x^2 - y'(x)/x = 0,$$

i.e., $2\Omega = xy(x) - x^2y'(x)$.

Let $f(x) = xy(x) - x^2y'(x)$. Since $y > 0$ and $y' < 0$, $f \geqslant 0$. Because of y's asymptotic behavior, $f(0) = 0$, $f'(0) = 1$, and $\lim_{x \to \infty} f(x) = 0$. f's behavior for large and small x can be described more exactly as need be. Our simple observations give the following incomplete picture:



The following lemma clears things up.

LEMMA. *f has exactly one critical point $\bar{x}$ and $f''(\bar{x}) < 0$.*

Proof of Lemma. We use Sommerfeld's analysis of the solution $y(x)$. (See [7].) He uses the following change of variables:

$$u = x^3y(x)$$

$$e^t = x$$

$$v = \frac{du}{dt}.$$

The T-F equation $y'' = y^{3/2}x^{-1/2}$ becomes

$$\frac{du}{dt} = v$$

$$\frac{du}{dt} = 7v + u(u^{1/2} - 12).$$

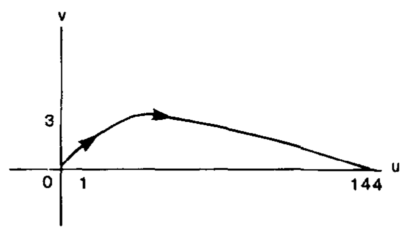
This equation has two singularities, at $(u, v) = (0, 0)$ and $(144, 0)$. Along a trajectory,

$$\frac{dv}{du} = 7 + \frac{u}{v}(u^{1/2} - 12).$$

By linearizing about the singularities, Sommerfeld shows that the trajectory $(u, v)(t)$ which corresponds to the solution $y(x)$ with $y(0)=1$ and $y(x)\approx 144x$ as $x\to\infty$ must satisfy

$$\left.\frac{dv}{du}\right|_{u=0}=3, \qquad \left.\frac{dv}{du}\right|_{u=144}=\frac{7-\sqrt{13}}{2}.$$

Furthermore, $v>0$. The trajectory looks like



In our new variables,

$$\begin{aligned} f'(x) &= y(x)-xy'(x)-x^2y''(x)\\ &= x^{-3}\left[u-v+3u-\frac{dv}{dt}+7v\ 12u\right]\\ &= x^{-3}\left[-8u+6v-\frac{dv}{dt}\right]. \end{aligned}$$

Hence, $f'(x)=0$ holds if and only if

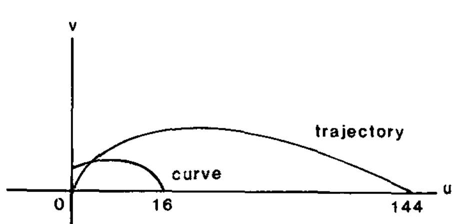
$$\frac{dv}{dt}=-8u+6v.$$

Since $dv/dt=7v+u(u^{1/2}-12)$, this implies

$$-8u+6v=7v+u^{3/2}-12u,$$

i.e., $v=u(4-u^{1/2})$.

Let us prove that this curve intersects the trajectory exactly once. Since the slope of our trajectory is 3 at the origin and the slope of $v=u(4-u^{1/2})$ is 4, it is obvious that the trajectory must intersect the curve at least once:



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At this point $du/dv|_{\text{trajectory}} \geqslant du/dv|_{\text{curve}}$. Notice that the slope of the trajectory and the curve at a point of intersection equal

$$7+\frac{(u^{1/2}-12)}{4-u^{1/2}} \qquad \text{and} \qquad 4-3/2u^{1/2},$$

respectively. The condition $du/dv|_{\text{trajectory}} \geqslant du/dv|_{\text{curve}}$ means $u^{1/2} \leqslant 8/3$.

Let us entertain the possibility that the trajectory touches the curve at more than one point. At the first point, $u^{1/2} \leqslant 8/3$. If the trajectory touches at another larger value of u then it must be that

$$\left.\frac{dv}{du}\right|_{\text{trajectory}} \leqslant \left.\frac{dv}{du}\right|_{\text{curve}}$$

Hence, $u^{1/2} \geqslant 8/3$ at this point. If $u^{1/2} > 8/3$ then

$$\left.\frac{dv}{du}\right|_{\text{trajectory}} < \left.\frac{dv}{du}\right|_{\text{curve}}.$$

For the trajectory to converge on (144, 0), it must cross the trajectory a third time (at a larger u) and satisfy

$$\left.\frac{dv}{du}\right|_{\text{trajectory}} > \left.\frac{dv}{du}\right|_{\text{curve}}.$$

But this would imply $u^{1/2} < 8/3$, a contradiction. The only possibility for a second contact point is that it be a point of tangency. That is, $u^{1/2} = 8/3$. Furthermore, it must be that

$$\left.\frac{d^2v}{du^2}\right|_{\text{trajectory}} > \left.\frac{d^2v}{du^2}\right|_{\text{curve}}.$$

(Or get the contradictory third contact point.) Let us calculate these derivatives. When $u^{1/2} = 8/3$ along the curve,

$$\begin{aligned} v &= u(4-u^{1/2}) \\ &= 64/9(4-8/3) = 256/27. \end{aligned}$$

$$\begin{aligned}
\left.\frac{d^2v}{du^2}\right|_{\text{trajectory}} &= \frac{d}{du}\,7+\frac{u}{v}\,(u^{1/2}-12)\\
&= -\frac{1}{v^2}\cdot\frac{dv}{du}\cdot u(u^{1/2}-12)+\frac{1}{v}\cdot[3/2u^{1/2}-12)\\
&= -\frac{1}{v^2}\left[7+\frac{u}{v}\,(u^{1/2}-12)\right]\cdot u(u^{1/2}-12)+\frac{1}{v}\,(3/2u^{1/2}-12)\\
&= -27/42;\\
\left.\frac{d^2v}{du^2}\right|_{\text{curve}} &= \frac{d}{du}\,(4-3/2u^{1/2})\\
&= 3/4u^{-1/2} = -9/32.
\end{aligned}$$

Hence, $d^2v/du^2|_{\text{trajectory}} < d^2v/du^2|_{\text{curve}}$ and we see that there cannot be a second crossing.

To prove that $f''(\bar{x})<0$, we write f'' in terms of u and v and calculate

$$\begin{aligned}
f''(x) &= \frac{d}{dx}\,[y(x)-xy'(x)-x^{3/2}y^{3/2}]\\
&= -xy''-3/2x^{1/2}\,y^{3/2}-3/2x^{3/2}\,y^{1/2}y'\\
&= -5/2x^{1/2}\,y^{3/2}-3/2x^{3/2}\,y^{1/2}y'\\
&= -x^{1/2}y^{1/2}(5/2y+3/2xy')\\
5/2y+3/2xy' &= 5/2ux^{-3}+3/2(vx^{-3}-3ux^{-3})\\
&= x^{-3}(3/2v-2u).
\end{aligned}$$

When $f'(x)=0$, $v=4u-u^{3/2}$. Hence, $3/2v-2u=47-3/2u^{3/2}=47(1-3/8u^{1/2})$. We have shown above that for $u^{1/2}<3/8$ that $f'(x)=0$. Hence, $f''(\bar{x})>0$. ∎

COROLLARY 1. *Let $0<\Omega<\bar{\Omega}$. $p(x)$ has exactly two critical points, the two solutions to $f(x)=2\Omega$. Let the first be denoted $x_c(\Omega)$, the second $x_m(\Omega)$. Then $p(x_c(\Omega))=-\mathscr{E}(\Omega)<0$ and $p(x_m(\Omega))>0$.*

Proof of Corollary 1. Clear. ∎

The following technical corollary will be useful later. Let $x_1(\Omega)<x_2(\Omega)$ be the two solutions of $\Omega/x^2=y(x)/x$.

COROLLARY 2. *Let $\varepsilon>0$. Given $\varepsilon<\Omega<\bar{\Omega}$, there are constants $c_i(\varepsilon)>0$ for which*

(i) $c_0(\varepsilon) < p''(x_c(\Omega))$.

(ii) *For* $x \in [\Omega/10, 2x_2(\Omega)]$, $|(d^k/dx^k)p(x)| < c_k(\varepsilon)$ *for* $k = 1, 2, 3$.

(iii) *For* $x \in [\Omega/10, x_c(\Omega) - c_3(\varepsilon)\, c_0(\varepsilon)^{-1}/10]$, $p'(x) < -c_4(\varepsilon)$.

(iv) *For* $x \in [x_c(\Omega) + c_3(\varepsilon)\, c_0(\varepsilon)^{-1}/10,\ (x_2(\Omega) + x_m(\Omega))/2]$, $p'(x) > c_4(\varepsilon)$.

(v) *For* $|x - x_c(\Omega)| < c_3(\varepsilon)\, c_0(\varepsilon)^{-1}/10$, $p(x) + \mathscr{E}(\Omega) = \frac{1}{2}(x - x_c(\Omega))^2$ *within a factor* $1 \pm 1/10$.

Proof of Corollary 2. Let $2\bar{\bar{\Omega}} \equiv \max_x f(x) = f(\bar{x})$. Since $[\Omega/x^2 - y(x)/x](x_m(\Omega)) > 0$ for all Ω and $x_c(\bar{\bar{\Omega}}) = x_m(\bar{\bar{\Omega}})$,

$$\min_x \{\bar{\bar{\Omega}}/x^2 - y(x)/x\} > 0.$$

Hence $\bar{\Omega} < \bar{\bar{\Omega}}$. Let $\bar{\bar{\Omega}} - \bar{\Omega} = \bar{c}$. Let $\varepsilon < \omega < \bar{\Omega}$ and, as usual,

$$p(x) = [\Omega/x^2 - y(x)/x].$$

Since all derivatives of y and hence of f are bounded for x near $\bar{x}$, $f(x)$ is given by $f(x) - 2\bar{\bar{\Omega}} = (1/2)(x - \bar{x})^2 f''(\bar{x})$ within a factor $(1 \pm 1/10)$ for x near enough to $\bar{x}$. Since $f''(\bar{x}) < 0$ and $2\bar{\bar{\Omega}} - 2\Omega > 2\bar{\bar{\Omega}} - 2\bar{\Omega} = 2\bar{c} > 0$, the solutions $x_c(\Omega)$ and $x_m(\Omega)$ to $f(x) = 2\Omega$ are at least some small distance $c = O(\bar{c}^{1/2} f''(\bar{x})^{-1/2})$ to the left and right of $\bar{x}$.

By definition,

$$p'(x) = \frac{f(x) - 2\Omega}{x^3}$$

$$p''(x) = \frac{f'(x)}{x^3} - \frac{3(f(x) - 2\Omega)}{x^4}.$$

As $f'(x) = (x - \bar{x})f''(\bar{x})$ within a factor $1 \pm 1/10$ for x near $\bar{x}_0$ and $x_c(\Omega) - \bar{x} < -c$, statement (i) follows. For $\varepsilon < \Omega < \bar{\Omega}$, $[\Omega/10, 2x_2(\Omega)]$ is contained in a finite region of the x-axis where all derivatives are bounded. Hence, (ii). Since $f(x)$ is monotone increasing for $x < \bar{x}$, the above expression for p' implies (iii). To prove (iv), notice that the difference $x_m(\Omega) - x_2(\Omega)$ is uniformly bounded below for $\varepsilon < \Omega < \bar{\Omega}$. (It is continuous in Ω and positive for all $\Omega \in [\varepsilon, \bar{\Omega}]$.) Hence, $(x_m(\Omega) + x_2(\Omega))/2$ is always less than $x_m(\Omega)$ minus some small constant. This means any $x \in [x_c(\Omega) + c_0 c_3^{-1}/100,\ (x_m(\Omega) + x_2(\Omega))/2]$ is at least a constant to the right of $x_c(\Omega)$, but less than a constant to the left of $x_m(\Omega)$. Since $x_c(\Omega)$ and $x_m(\Omega)$ lie to the left and right, respectively, of $x_c(\bar{\Omega})$ and $x_m(\bar{\Omega})$, $f'(x)$ is bounded away from zero there. This implies that f is some small constant larger than 2Ω in the region under consideration. Hence, (iv). Statement (v) follows from (ii) by Taylor's Theorem. ∎

Before specializing to our special potential, let us develop WKB approximations in a general setting. Consider

$$w''(x) - \lambda^2 p(x)\, w(x) = 0, \tag{II.1}$$

where $\lambda > 0$ is a large parameter and $p(x)$ is a smooth function defining a potential well. By "potential well," we mean

(i) There are two points $x_1 < x_2$ called "turning points" of p, at which p is zero and $p(x) < 0$ for $x \in (x_1, x_2)$, $p(x) > 0$ for $x \notin [x_1, x_2]$.

(ii) There is exactly one critical point $x_c \in (x_1, x_2)$. At this point $p''(x_c) > 0$.

For large values of λ, solutions of (II.1) can be closely approximated by functions that are amenable to explicit calculations. This allows us to solve boundary value problems for (II.1) to high accuracy.

When $p(x) > 0$, solutions to (II.1) are well approximated by exponentials of $\pm\lambda \int^x p(t)^{1/2}\, dt$ and when $p(x) < 0$, by sines and cosines of $\pm\lambda \int^x |p(t)|^{1/2}\, dt$. To be a little more precise,

$$\bar{u}_{1,2} = p(x)^{-1/4} \exp\left[\pm\lambda \int^x p(t)^{1/2}\, dt \right] \tag{II.2}$$

approximately solves (1) when $p > 0$, and

$$\begin{aligned} \bar{v}_1(x) &= |p(x)|^{-1/4} \cos\left[\lambda \int^x |p(t)|^{1/2}\, dt \right] \\ \bar{v}_2(x) &= |p(x)|^{-1/4} \sin\left[\lambda \int^x |p(t)|^{1/2}\, dt \right] \end{aligned} \tag{II.3}$$

approximately solves (II.1) when $p < 0$. In Lemmas 1 and 2, we calculate the accuracy of the approximations by using the Green's function. We then discuss the errors involved in using the approximations to solve boundary value problems. These errors are of order $1/\lambda$ for large λ and depend on the size of p and its derivatives.

A slightly more complicated problem arises when we try to approximate solutions in the neighborhood of the turning points. For x very close to a turning point x_i, $p'(x_i)(x - x_i)$ closely approximates $p(x)$. Accordingly, solutions to

$$w'' - \lambda^2 p'(x_i)(x - x_i)\, w(x) \tag{II.4}$$

closely approximate solutions to (II.1). Solutions to (II.4) are scaled Airy functions. As expected, when $\lambda^2 p'(x_i)(x - x_i) \gg 0$ these solutions look like those in (II.2) and when $\lambda^2 p'(x_i)(x-x_i) \leqslant 0$, like (II.3). In Lemma 3, we make this explicit. That is, we calculate how closely solutions to (II.4) approximate solutions to (II.1) near x_i and then use standard results about Airy functions to compare these solutions to (II.2) and (II.3) in the appropriate regions.

A central concept in solving boundary value problems is the "phase" of a solution w. The phase is defined as

$$\mathcal{O}[w](x) = \frac{(w'(x), w(x))}{\sqrt{|w'|^2 + |w|^2}}.$$

It is a point on the unit circle. Notice that if $w(x) = \bar{w}(x) + \varepsilon(x)$ and

$$(|\varepsilon(x)| + |\varepsilon'(x)|) < \delta(|\bar{w}(x)| + |\bar{w}'(x)|),$$

with $0 < \delta < 1/10$ (say), then

$$|\mathcal{O}[w](x) - \mathcal{O}[\bar{w}](x)| < 2\delta.$$

Lemmas 1, 2, 3 below estimate the $\varepsilon(x)$ by which the solution w to (II.1) differs from the approximate solutions $\bar{w}$ given above and allow an estimate on δ. This will allow us to calculate how $\mathcal{O}[w](x)$ changes with c.

LEMMA 1. *Let $a < b$ and suppose $p(x) > 0$ on $[a, b]$. Let $\eta(x) = \int_a^x p^{1/2}(t)\, dt$ and define*

$$\bar{u}_{1,2}(x) = p(x)^{-1/4} \exp[\pm \lambda \eta(x)].$$

Let $A = \int_a^b (|p'|^2 |p|^{-5/2} + |p''|\, |p|^{-3/2})\, dx$. Assume $\lambda > 10A$ and $\lambda > 2|p(x)^{-1/4}\, d/dx\, p(x)^{-1/4}|$ for all $x \in [a, b]$. Then, there are solutions $u_i = \bar{u}_i + \varepsilon_i$ $(i = 1, 2)$ to (1) for which

$$(|\varepsilon_i(x)| + |\varepsilon_i'(x)|) < 5A/\lambda(|\bar{u}_i(x)| + |\bar{u}_i'(x)|)$$

for all $x \in [a, b]$.

Proof of Lemma 1. Let $u_1 = \bar{u}_1 + \varepsilon_1$ be a solution of (II.1) on $[a, b]$ with $\varepsilon_1(a) = \varepsilon_1'(a) = 0$ and let $u_2 = \bar{u}_2 + \varepsilon_2$ be a solution with $\varepsilon_2(b) = \varepsilon_2'(b) = 0$. We will prove

$$(|\varepsilon_i(x)| + |\varepsilon_i'(x)|) < (5A/\lambda)(|\bar{u}_i(x)| + |\bar{u}_i'(x)|). \tag{II.5}$$

Let us deal with $i = 1$. The case $i = 2$ is handled in the same way.

Direct computation shows

$$\bar{u}_1'' - (\lambda^2 p(x) - \delta(x))\, \bar{u}_1(x) = 0, \tag{II.6}$$

where $\delta(x) = (5/16)(p'/p)^2 - (1/4)(p''/p)$. Since w_+ satisfies Eq. (II.1), ε_1 satisfies

$$\varepsilon_1'' - \{\lambda^2 p(x) - \delta(x)\}\, \varepsilon_1(x) = \delta(x)(\bar{u}_1(x) + \varepsilon_1(x)). \tag{II.7}$$

The Green's function for (II.6) is

$$K(x, t) = (1/2\lambda)(\bar{u}_1(x)\, \bar{u}_2(t) - \bar{u}_1(t)\, \bar{u}_2(x))$$

for $t < x$ and zero for $t > x$. By (II.7) and the boundary condition for ε_1 at $x = a$,

$$\varepsilon_1(x) = \int_a^x K(x, t)\, \delta(t)(\bar{u}_1(t) + \varepsilon_1(t))\, dt.$$

Let $\bar{\varepsilon}(x) = \varepsilon_1(x)/\bar{u}_1(x)$. The above equation can be rewritten

$$\bar{\varepsilon}(x) = (1/2\lambda) \int_a^x F(x, t)\, \delta(t)(1 + \bar{\varepsilon}(t))\, dt, \tag{II.8}$$

where $F(x, t) = (1 - \exp[2\lambda(\eta(t) - \eta(x))])\, p(t)^{-1/2}$. Equation (II.8) can be solved formally by recursion to yield

$$\begin{aligned}\bar{\varepsilon}(x) = \sum_{k=1}^{\infty} (1/2\lambda) \iint_{x > t_1 > \cdots > t_K > a} & dt_1 \cdots dt_k \\ & \times \{F(x, t_1) \cdots F(t_{k-1}, t_k) \cdot \delta(t_1) \ldots \cdot \delta(t_k)\}.\end{aligned} \tag{II.9}$$

Since $x > t_1 > \cdots > t_k > a$, the jth F factor has absolute value less than $p(t_j)^{-1/2}$. Since the k-dimensional volume of $\{x > t_1 > \cdots > t_k > a\}$ equals $[a, x]^k/k!$, the kth term in (II.9) has absolute value

$$\begin{aligned}&\leqslant (1/2\lambda)(1/k!) \left(\int_a^x |\delta(t)|\, p(t)^{-1/2}\, dt \right)^k \\ &\leqslant (A/\lambda)^k\, (1/k!).\end{aligned}$$

Hence, the sum converges to a limit $\bar{\varepsilon}(x)$ which satisfies (II.8). Also

$$|\bar{\varepsilon}(x)| \leqslant \exp[A/\lambda] - 1.$$

Since $A/\lambda < 1/10$,

$$|\bar{\varepsilon}(x)| < (A/\lambda).$$

Now differentiate Eq. (II.8):

$$\bar{\varepsilon}'(x) = 4p(x)^{1/2} \int_a^x \exp[2\lambda(\eta(t) - \eta(x))] \cdot \delta(t)\, p(t)^{-1/2} (1 + \bar{\varepsilon}(t))\, dt. \tag{II.10}$$

Hence, $|\bar{\varepsilon}'(x)| < 2p(x)^{1/2} A$. By definition,

$$\varepsilon_1'(x) = \bar{\varepsilon}(x)\, \bar{u}_1'(x) + \bar{\varepsilon}'(x)\, \bar{u}_1(x).$$

Hence, $|\varepsilon_1'(x)| < (A/\lambda)|\bar{u}_1'(x)| + 2Ap(x)^{1/2}\, \bar{u}_1(x)$. Since

$$\bar{u}_1'(x) = \left\{ p(x)^{1/4} \frac{d}{dx} p(x)^{-1/4} + \lambda p(x)^{1/2} \right\} \bar{u}_1$$

and

$$\lambda < 2 \left| p(x)^{-1/4} \frac{d}{dx} p(x)^{-1/4} \right|,$$

$$|\varepsilon_1'(x)| < (5A/\lambda)|\bar{u}_1'(x)|. \quad \blacksquare$$

LEMMA 2. *Let* $a < b$ *and suppose* $p(x) < 0$ *on* $[a, b]$. *Let* $\eta(x) = \int_a^x |p|^{1/2}(t)\, dt$ *and define*

$$\bar{v}_1(x) = |p(x)|^{-1/4} \cos[\lambda\eta(x)]$$

$$\bar{v}_2(x) = |p(x)|^{-1/4} \sin[\lambda\eta(x)].$$

Let $B = \int_a^b (|p'|^2\, |p|^{-5/2} + |p''|\, |p|^{-3/2}\, dx$. *Assume* $\lambda > 10B$ *and* $\lambda > 2\, |\, |p(x)|^{-1/4} (d/dx)\, |p(x)|^{-1/4}|$ *for all* $x \in [a, b]$. *Then, there are solutions* v_1 *and* v_2 *to* (II.1) *so that for all* $x \in [a, b]$

$$\begin{pmatrix} v_i \\ v_i' \end{pmatrix}(x) = c_1^i \begin{pmatrix} v_i \\ \bar{v}_1' \end{pmatrix}(x) + c_2^i \begin{pmatrix} \bar{v}_2 \\ \bar{v}_2' \end{pmatrix}(x)$$

for some c_1^i, c_2^i *(depending on* x*) with* $|c_1^1 - 1|, |c_2^2 - 1|, |c_1^2|, |c_2^1|$ *all* $< 5A\lambda$.

Proof of Lemma 2. As in the proof of Lemma 1, we have an expression for the error ε_1:

$$\varepsilon_1(x) = \int_a^x K(x, t)\, \delta(t)(\bar{v}_1(t) + \varepsilon_1(t))\, dt. \tag{II.11}$$

Whereas the exponentials complicated matters in Lemma 1, we can use a simple bound

$$|K(x, t)| < (1/2\lambda)\, |p(x)|^{-1/4}\, |p(t)|^{-1/4}$$

to estimate $|\varepsilon_1(x)|$ directly. That is, do the recursion and find

$$|\varepsilon_1(x)| < (B/\lambda)|p(x)|^{-1/4}.$$

Upon differentiating (II.11) (i.e., replacing $K(x, t)$ by $(\partial/\partial x)\, K(x, t)$) and using the assumption that

$$\lambda > 2 \left| |p(x)|^{-1/4} \frac{d}{dx} |p(x)|^{-1/4} \right|,$$

we find $|\varepsilon_1'(x)| < 4B|p(x)|^{1/4}$.

Proving the conclusion of Lemma 2 is slightly more tricky. Since $\bar{v}_1$ and $\bar{v}_2$ are linearly independent functions, we know that given x, there are constants $c_1^1(x)$ and $c_2^1(x)$ so that

$$v_1(x) = c_1^1 \bar{v}_1(x) + c_2^1 \bar{v}_2(x)$$
$$v_1'(x) = c_1^1 \bar{v}_1'(x) + c_2^1 \bar{v}_2'(x).$$

Subtracting $\bar{v}_1$ from the first equation and $\bar{v}_1'$ from the second gives

$$\begin{aligned} \varepsilon_1(x) &= (c_1^1 - 1)\, \bar{v}_1(x) + c_2^1 \bar{v}_2(x) \\ \varepsilon_1'(x) &= (c_1^1 - 1)\, \bar{v}_1(x) + c_2^1 \bar{v}_2'(x). \end{aligned} \tag{II.12}$$

For notational convenience, let $v, v_\perp \in \mathbb{R}^2$ be the vectors

$$v = \begin{pmatrix} \cos[\lambda \int_a^x |p|^{1/2}] \\ \sin[\lambda \int_a^x |p|^{1/2}] \end{pmatrix}$$
$$v_\perp = \begin{pmatrix} -\sin[\lambda \int^x |p|^{1/2}] \\ \cos[\lambda \int_a^x |p|^{1/2}] \end{pmatrix}.$$

Note that v and $v_\perp$ are orthogonal unit vectors. From (II.12), the definitions of $\bar{v}_{1,2}$, and the estimates on ε_1 and ε_1' just proved, we have

$$|(c_1^1 - 1, c_2^1) \cdot v| < B/\lambda$$
$$|(c_1^1 - 1, c_2^1) \cdot v| < B/\lambda. \quad \blacksquare$$

For Lemma 3, we need to discuss the Airy functions $A_1(x)$ and $A_2(x)$ defined below. For a more complete analysis, see Erdélyi's excellent little book [8]. Consider the Airy equation

$$y''(x) - xy(x) = 0. \tag{II.13}$$

Equation (II.13) has two linearly independent solutions $A_1(x)$ and $A_2(x)$

which are bounded with bounded derivatives on $[-1, 1]$ and have asymptotic behavior given by

$$\begin{aligned}
A_1(x) &= x^{-1/4}\exp[-(2/3)\,x^{3/2}]\cdot\{1+\varepsilon_1(x)\}, && x>1\\
A_1(x) &= 2|x|^{-1/4}\cos[(2/3)\,|x|^{3/2}-\pi/4]+\tilde{\varepsilon}_1(x), && x<-1\\
A_2(x) &= x^{-1/4}\exp[(2/3)\,x^{3/2}]\cdot\{1+\varepsilon_2(x)\}, && x>1\\
A_2(x) &= 2|x|^{-1/4}\cos[(2/3)\,|x|^{3/2}+\pi/4]+\tilde{\varepsilon}_2(x), && x<-1,
\end{aligned} \tag{II.14}$$

where

$$|\varepsilon_i(x)| < \tilde{K}x^{-3/2}, \qquad |\varepsilon_i'(x)| < \tilde{K}x^{-3/2},$$
$$|\tilde{\varepsilon}_i(x) < \tilde{K}|x|^{-7/4}, \qquad |\tilde{\varepsilon}_i'(x)| < \tilde{K}|x|^{-7/4}.$$

The fact that solutions to (II.13) are given by $|x|^{-1/4}$ times exponentials for $x>1$ and $|x|^{-1/4}$ times sines and cosines for $x<-1$ modulo errors obeying the above bounds follows directly from Lemmas 1 and 2 with $p(x)=x$. Equation (II.14) gives the relationship between the asymptotic forms to the left and right of zero. It can be reduced to the analogous problem for Bessel functions, where results are well known. See [8] for details.

LEMMA 3. *Let $p(c)=0$, $p'(c)<0$, and ε small enough that*

$$\varepsilon \max_{|x-c|<\varepsilon} |p''(x)/p'(x)| < 1/100$$
$$\varepsilon^2 \max_{|x-c|<\varepsilon} |p'''(x)/p'(x)| < 1/100.$$

Let $C=\varepsilon^{-3/2}\,|p'(c)|^{-1/2}$. Let $\tilde{K}$ be the constant associated to the uniform Airy function asymptotically. Assume $\lambda > \tilde{K}\cdot C$. Also, assume $\lambda > 2|p|^{-1/4}\,|(d/dx)\,|p|^{-1/4}|$ for $|x-c|>\varepsilon/2$. Let

$$\begin{aligned}
\bar{w}_1(x) &= p(x)^{-1/4}\exp\left[-\lambda\int_x^c p(t)^{1/2}\,dt\right] && \textit{if} \quad x<c-\varepsilon/2\\
&= 2|p(x)|^{-1/4}\cos\left[\lambda\int_c^x |p(t)|^{1/2}\,dt-\pi/4\right] && \textit{if} \quad x>c+\varepsilon/2;\\
\bar{w}_2(x) &= p(x)^{-1/4}\exp\left[\lambda\int_x^c p(t)^{1/2}\,dt\right] && \textit{if} \quad x<c-/2\\
&= 2|p(x)|^{-1/4}\cos\left[\lambda\int_c^x |p(t)|^{1/2}\,dt+\pi/4\right] && \textit{if} \quad x>c+\varepsilon/2.
\end{aligned}$$

Then, there are solutions w_i $(i=1,2)$ to (II.1) *on* $[c-\varepsilon, c+\varepsilon]$ *satisfying*

$$(|w_i-\bar{w}_i|(x)+|w_i'-\bar{w}_i'|)(x)<(K\cdot C/\lambda)(|\bar{w}_i|+|\bar{w}_i'|)(x) \qquad \text{(II.15)}$$

if $x<c-\varepsilon/2$, *and if* $x>c+\varepsilon/2$

$$\begin{pmatrix} w_i \\ w_i' \end{pmatrix}(x)=c_1^i(x)\begin{pmatrix} \bar{w}_1 \\ \bar{w}_1' \end{pmatrix}(x)+c_2^i(x)\begin{pmatrix} \bar{w}_2 \\ \bar{w}_2' \end{pmatrix}(x)$$

with $|c_1^1-1|$, $|c_2^2-1|$, $|c_1^2|$, $|c_2^1|$ *all* $<\tilde{K}\cdot c/2\lambda$.

Proof of Lemma 3. Let

$$\xi(x)=\left[(3/2)\int_x^c p(t)^{1/2}\,dt\right]^{2/3} \qquad \text{if} \quad x\leqslant c,$$

$$\xi(x)=-\left[(3/2)\int_c^x |p(t)|^{1/2}\,dt\right]^{2/3} \qquad \text{if} \quad x\geqslant c.$$

Let

$$\tilde{w}_1(x)\lambda^{1/6}[-\xi'(x)]^{-1/2}A_1(\lambda^{2/3}\xi(x))$$
$$\tilde{w}_2(x)=\lambda^{1/6}\lfloor-\xi'(x)\rfloor^{-1/2}A_2(\lambda^{2/3}\xi(x)).$$

By (II.14), $\tilde{w}_i$ have asymptotic forms $\bar{w}_i$, where $\bar{w}_i$ is defined in the statement of this lemma. The errors between $\tilde{w}_i$ and $\bar{w}_i$ for $|x-c|>\varepsilon/2$ obey the bounds on ε_i and $\tilde{\varepsilon}_i$ in (II.14), with $|x|$ replaced by $\lambda^{2/3}\xi(x)$. That is,

$$|\tilde{w}_i-\bar{w}_i|(x)<\tilde{K}\left(\lambda\int_x^c p(t)^{1/2}\,dt\right)^{-1}|\bar{w}_i(x)|$$

$$|\tilde{w}_i'-\bar{w}_i'|(x)<2\tilde{K}\left(\lambda\int_x^c p(t)^{1/2}\,dt\right)^{-1}|\bar{w}_i'(x)|$$

when $x<c-\varepsilon/2$, and

$$|\tilde{w}_i-\bar{w}_i|(x)<\tilde{K}\left(\lambda\int_c^x |p(t)|^{1/2}\,dt\right)^{-1}|p(x)|^{-1/4}$$

$$|\tilde{w}_i'-\bar{w}_i'|(x)<\tilde{K}\left(\lambda\int_c^x |p(t)|^{1/2}\,dt\right)^{-1}\lambda|p(x)|^{1/4}$$

when $x>c+\varepsilon/2$. Notice that within a factor of two

$$\int_x^c p(t)^{1/2}\,dt \qquad \text{and} \qquad \int_c^x |p(t)|^{1/2}\,dt \qquad \text{equal} \qquad p'(c)^{1/2}\,\varepsilon^{3/2}.$$

On the other hand, $\tilde{w}_i$ closely approximate solutions to (II.1) over the entire interval $[c-\varepsilon, c+\varepsilon]$. Direct computation shows

$$\tilde{w}_i'' - (\lambda^2 p(x) - \delta(x))\, \tilde{w}_i(x) = 0, \tag{II.16}$$

where $\delta(x) = \xi'''/\xi' - (3/2)(\xi''/\xi')^2$. Noting that $\xi'(x) = -|p|^{1/2}\,|\xi|^{-1/2}(x)$, it is easy to calculate that

$$\delta(x) = (1/2)(p''/p) + (5/8)(p\xi^{-3} - (p'/p)^2).$$

Using our assumption on ε, we have

$$p(x) = p'(c)(x-c) + 1/2 p''(c)(x-c)^2 + O(\varepsilon^2 p'(c)^{-1}(x-x_c)^3).$$

Using this expression, we can calculate

$$|\delta(x)| < (1/100)\,\varepsilon^{-2}.$$

As in Lemmas 1 and 2 we write solutions w_i to (II.1) as $w_i = \tilde{w}_i + \varepsilon_i$ and apply the Green's function to estimate ε_i and ε_i'. We use the estimates (II.14) and the fact that Airy's functions are bounded with bounded first derivatives on bounded intervals. Let $\varepsilon_1(c-\varepsilon) = \varepsilon_1'(c-\varepsilon) = 0$. Then,

$$\varepsilon_1(x) = (1/2\lambda) \int_{c-\varepsilon}^{x} [\tilde{w}_1(x)\,\tilde{w}_2(t) - \tilde{w}_1(t)\,\tilde{w}_2(x)] \cdot \delta(t) \cdot [\tilde{w}_1(t) + \varepsilon_1(t)]\, dt.$$

Since $\tilde{w}_i$ has asymptotic form $\bar{w}_i$ in $[c-\varepsilon_1, c-\varepsilon/2\rfloor$, the same analysis as in Lemma 1 implies that

$$|\varepsilon_1(x)| < (1/2\lambda) \int_c^x |\delta(t)|\, |p(t)|^{-1/2}\, dt \cdot |w_1(x)|$$

and

$$|\varepsilon_1'(x)| < (2/\lambda) \int_{c-\varepsilon}^{x} |\delta(t)|\, |p(t)|^{-1/2}\, dt \cdot |w_1'(x)|.$$

Since $|\delta(t)| < 1/100\varepsilon^{-2}$ and $p(t) = p'(c)(t-c)$ within a small factor, we find

$$\left| \int_{c-\varepsilon}^{x} |\delta(t)|\, |p(t)|^{-1/2}\, dt \right| < 1/100\varepsilon^{-3/2} |p'(c)|^{-1/2}$$

as desired. When $x > c + \varepsilon/2$, we break the integral into three parts. Let $\bar{\varepsilon}$ be a small number defined for each λ by

$$\lambda \int_{c-\bar{\varepsilon}}^{c+\bar{\varepsilon}} |p(t)|^{1/2}\, dt = \text{ large fixed constant.}$$

Because of our original choice of λ as greater than $\tilde{K} \cdot C$, we may assume $\bar{\varepsilon} < \varepsilon/2$ for all λ. Furthermore, notice that

$$\bar{\varepsilon} = \lambda^{-2/3} |p'(c)|^{-1/3}$$

within a factor which is independent of λ.

Recalling $K(x, t) = (1/2\lambda)[\tilde{w}_1(x)\, \tilde{w}_2(t) - \tilde{w}_1(t)\, \tilde{w}_2(x)]$ and the asymptotic form $\tilde{w}_i(x)$ of (II.14) when $x > c + \varepsilon/2$, we have

$$|K(x, t)| < (1/2\lambda) |p|^{-1/4}(x) [|\tilde{w}_1(t)| + |\tilde{w}_2(t)|].$$

To apply the recursive argument of Lemmas 1 and 2, we estimate

$$\int_{c-\varepsilon}^{c+\varepsilon} [|\tilde{w}_1|(t) + |\tilde{w}_2(t)|]\, |\delta(t)|\, |\tilde{w}_1(t)|\, dt$$
$$= \int_{c-\varepsilon}^{c-\bar{\varepsilon}} + \int_{c-\bar{\varepsilon}}^{c+\bar{\varepsilon}} + \int_{c+\bar{\varepsilon}}^{x}.$$

The asymptotic forms (II.14) imply that for $|x - c| > \bar{\varepsilon}$, $|\tilde{w}_1|^2$ and $|\tilde{w}_1|\, |\tilde{w}_2|$ are both $\leqslant |p(t)|^{-1/2}$. Hence, their contribution is bounded by

$$\int_{c-\varepsilon}^{c+\varepsilon} |\delta(t)|\, |p(t)|^{-1/2}\, dt < \varepsilon^{-3/2} |p'(c)|^{-1/2}.$$

The second integral can be calculated by using the uniform bound on A_1 and A_2 when their argument

$$\pm \left[\lambda(3/2) \int_x^c |p|^{1/2}\, dt \right]^{3/2}$$

is bounded. Also, recall that $p(x)$ is given within a factor $1 \pm 1/100$ by $p'(c)(x - c)$ when $|x - c| < \varepsilon$ and that $\lambda > (\text{large const.}) \cdot p'(c)^{-1/2}\, \varepsilon^{-3/2}$. We find this contribution is also bounded by

$$\text{const. } p'(c)^{-1/2}\, \varepsilon^{-3/2}.$$

This proves the result for $\varepsilon_1(x)$.

To prove the result for $\varepsilon_1'(x)$ when $x > c + \varepsilon/2$, notice that

$$\varepsilon_1'(x) = \int_{c-\varepsilon}^{x} \frac{\partial}{\partial x} K(x, t)\, \delta(t) (\tilde{w}_1(t) + \varepsilon_1(t))\, dt.$$

Using the asymptotic form (II.14) and the assumption $\lambda > 2|p|^{-1/4}\,|(d/dx)|\,|p|^{-1/4}$ when $x > c + \varepsilon/2$, we find

$$\left|\frac{\partial}{\partial x} K(x, t)\right| < |p|^{1/4}(x)[|\tilde{w}_1(t)| + |\tilde{w}_2(t)|].$$

The same estimates as above now prove the result for $\varepsilon_1'(x)$.

The result for ε_2 and ε_2' is proved in exactly similar fashion. That is, let $\varepsilon_2(c+\varepsilon) = \varepsilon_2'(c+\varepsilon) = 0$. Then

$$\varepsilon_2(x) = \int_x^{c+\varepsilon} K(x, t)\,\delta(t)(\tilde{w}_2(t) + \varepsilon_2(t))\,dt.$$

The estimates in $[c+\varepsilon/2, c+\varepsilon]$ are given by the asymptotic forms and the arguments of Lemma 2. The estimates in $[c-\varepsilon, c-\varepsilon/2]$ follow by breaking the integral up as we did for ε_1. ∎

These lemmas can help us find those values $\mathscr{E}_0 > \mathscr{E}_1 > \cdots > 0$ for which

$$w'' - Z^{2/3}[\Omega/x^2 - y(x)/x + \mathscr{E}_K] = 0 \tag{II.1'}$$

has a solution which is both finite at $x = 0$ and decays exponentially at $x = \infty$. We take a trial eigenvalue $\mathscr{E}$, establish a boundary condition for w at two points x_0 near zero and x_∞ near infinity, use our lemmas to extend w across intervals where $[\Omega/x^2 - y(x)/x + \mathscr{E}]$ is positive, negative, or zero, and then find a condition on $\mathscr{E}$ that makes the solution that we propagated forward from zero match with the solution propagated backward from infinity.

Let $x_1 < x_2$ be the turning points of $[\Omega/x^2 - y(x)/x + \mathscr{E}]$. Since $y(x) < 1$ and $\mathscr{E} > 0$, $x_1 > \Omega$. Let $x_0 = \Omega/10$. Let $x_\infty = (x_2(\Omega) + x_m(\Omega))/2$. (Recall Corollary 2). We calculate the boundary condition at $x = x_0$. Notice that since $[\Omega/x^2 - y(x)/x + \mathscr{E}] > (9/10)\Omega/x^2$ for $x < x_0$, the solution to (II.1') which is L^2 at the origin increases more rapidly than the corresponding solution to

$$w'' - Z^{2/3}(9/10)(\Omega/x^2)\,w = 0.$$

Its solutions are given by $w(x) = c_1 x^{s_1} + c_2 x^{s_2}$ where

$$s_1 = \frac{1 + \sqrt{1 + 4Z^{2/3}(9/10)\,\Omega}}{2}$$

$$s_2 = \frac{1 - \sqrt{1 + 4Z^{2/3}(9/10)\,\Omega}}{2}$$

are solutions to the indical equation

$$s(s-1)-Z^{2/3}(9/10)\,\Omega=0.$$

For w to behave correctly at $x=0$, $c_2=0$. This gives a boundary condition for our solution w to (II.1′):

$$\begin{pmatrix} w \\ w' \end{pmatrix}(\Omega/10)=\begin{pmatrix}\text{non-zero}\\ \text{constant}\end{pmatrix}\cdot\begin{pmatrix}1\\ \alpha_0\end{pmatrix} \tag{II.17}$$

with $\alpha_0 > s_1/(\Omega/10)$.

Recall from Section I (see (I.10)) that we use the WKB results when $\Omega > \Omega(Z) = L(Z)(L(Z)+1)\,Z^{-2/3} \approx Z^{-4/9} \gg Z^{-2/3}$. Hence

$$s_1/(\Omega/10)=Z^{1/3}\Omega^{-1/2}(9/10)+O(\Omega^{1/2}Z^{-1/3}).$$

For $x > x_\infty$, the constant $\mathscr{E}$ is a lower bound for our potential. The solution to

$$w''-Z^{2/3}\mathscr{E}w=0$$

which has the correct behavior at infinity is $w(x)=C\exp[-Z^{1/3}\sqrt{\mathscr{E}}\,x]$. It has boundary condition at x_∞ given by

$$\begin{pmatrix} w \\ w' \end{pmatrix}(x_\infty)=\begin{pmatrix}\text{non-zero}\\ \text{constant}\end{pmatrix}\cdot\begin{pmatrix}1\\ -\alpha_\infty\end{pmatrix} \tag{II.18}$$

with $\alpha_\infty > Z^{1/3}\sqrt{\mathscr{E}}$.

Given $\mathscr{E}$, we extend the solution w_0 satisfying (II.17) forward into the region where $p(x)$ is negative and we extend the solution w_∞ satisfying (II.18) backwards into the region where $p(x)$ is negative. We determine the values $\mathscr{E}_k$ for which the two agree.

Let us begin with w_0. We pick an interval $[x_1-\varepsilon_1, x_1+\varepsilon_1]$ about the left turning point x_1 on which we will apply Lemma 3. Equation (II.17) and Lemma 1 applied to $[x_0, x_1-\varepsilon_1]$ imply a boundary condition at $x_1-\varepsilon_1$. We pick ε_1 just small enough that the conditions of Lemma 3 hold:

$$\varepsilon_1 \max_{|x_1-x|<\varepsilon_1} |p''(x)|/|p'(x_1)| < 1/100$$

$$\varepsilon_1^2 \max_{|x_1-x|<\varepsilon_1} |p'''(x)|/|p'(x_1)| < 1/100.$$

All quantities depend on Ω and $\mathscr{E}$. Let us first consider arbitrary $\Omega \in [L(Z)(L(Z)+1)\,Z^{-2/3}, \bar{\Omega}]$ and $\mathscr{E}$ near enough to $\mathscr{E}(\Omega)$ that a quadratic approximation to p about the critical point x_c is appropriate for calculations around and between the critical points. When Ω is small, say

$\Omega < 10^{-2}$, we can use y's small x asymptotic form to calculate the critical point and the derivatives of p near it. When $\Omega > 10^{-2}$ we have uniform bounds given by Corollary 2. For $\Omega < 10^{-2}$, we use

$$1 - wx < y(x) < 1 - wx + 4/2\, x^{3/2}$$
$$-w < y'(x) < -w + 2x^{1/2}.$$

This follows from Section 0. Alternatively, it can be calculated by substituting the obvious inequality

$$1 - wx < y(x) < 1$$

into the T-F equation $y'' = y^{3/2} x^{-1/2}$ and then integrating. The critical point x_c solves

$$\frac{d}{dx}\left[\Omega x^{-2} - y(x)\, x^{-1}\right] = 0.$$

This implies $x_c(\Omega) = 2\Omega + O(\Omega^{5/2})$ for small Ω. Differentiating again, we find the second derivative $p''(x_c)$ equals $(2\Omega)^{-3}$ within a factor which is very close to 1 when $\Omega < 10^{-2}$. Furthermore, $|p''(x)|$ and $|p''(x)|$ are uniformly bounded by const. $\cdot\, \Omega^{-3}$ and const. $\cdot\, \Omega^{-4}$, respectively, when $x > \Omega/10$. By Corollary 2, we can adjust these constants in such a way that these estimates hold for all $\Omega < \bar{\Omega}$. That is,

$$\begin{aligned} &p''(x_c) > c\Omega^{-3}, \qquad \text{and} \\ &|p'(x)| < \bar{c}\Omega^{-2} \\ &|p''(x)| < \bar{c}\Omega^{-3} \\ &|p'''(x)| < \bar{c}\Omega^{-4} \end{aligned} \tag{II.19}$$

when $x \in [x_0(\Omega), x_\infty(\Omega)]$. For convenience, we write

$$p''(x_c) = c(\Omega)\, \Omega^{-3}$$

and note that $0 < c < c(\Omega) < \bar{c} < \infty$.

When $|\mathscr{E} - \mathscr{E}(\Omega)|$ is small enough, solutions to $p(x) = 0$ are well approximated by those to

$$\tfrac{1}{2} p''(x_c)(x - x_c)^2 + \mathscr{E} - \mathscr{E}(\Omega) = 0.$$

In fact,

$$(x_i - x_c) = \mp \sqrt{2(\mathscr{E}(\Omega) - \mathscr{E})\, p''(x_c)^{-1}}\, (1 + \alpha),$$
$$|\alpha| < \sqrt{\mathscr{E}(\Omega) - \mathscr{E}} \max_{x \in (x_1, x_2)} |p'''(x)|\, |p''(x_c)|^{-3/2}.$$

By (II.19), $|\alpha| < 10^{-3}$ as long as $|\mathscr{E}(\Omega) - \mathscr{E}| < (c^3 c^{-2} 10^{-6}) \cdot \Omega^{-1}$. Let $\mathscr{E}$ be in this range. Within one part in a thousand

$$\begin{aligned} |x_i - x_c| &= \sqrt{2(\mathscr{E}(\Omega) - \mathscr{E})\, c(\Omega)^{-1} \Omega^3}, \qquad \text{and} \\ p'(x) &= c(\Omega)\, \Omega^{-3}(x - x_c) \qquad \text{for all} \\ |x - x_c| &< 2|x_i - x_c|. \text{ Let } \mathscr{E}_i = 10^{-2}|x_1 - x_c|. \end{aligned} \tag{II.20}$$

Now solve the boundary value problem for w_0 on $[x_0, x_1 - \varepsilon_1]$. For Lemma 1 to apply here, $Z^{1/3}$ must be larger than both

$$\int_{x_0}^{x_1 - \varepsilon_1} (|p'|^2\, |p|^{-5/2} + |p''|\, |p|^{-3/2})$$

and

$$\sup \left\{ |p|^{-1/4} \left| \frac{d}{dx} |p|^{-1/4} \right| (x) \,\middle|\, x_0 < x < x_1 - \varepsilon_1 \right\}. \tag{II.21}$$

We picked $|\mathscr{E}(\Omega) - \mathscr{E}|$ small enough that the turning points x_1 and x_2 lie within the region where

$$[\Omega x^{-2} - y(x)\, x^{-1} + \mathscr{E}(\Omega)] = 1/2c(\Omega)\, \Omega^{-3}(x - x_c)^2 \tag{II.22}$$

within one part in a thousand. Define $\bar{x}_1 < x_c < \bar{x}_2$ by

$$|\bar{x}_i - x_c| = 10^{-2} c\, \bar{c}^{-1} \Omega.$$

By (II.10), (II.22) holds within 1/10 of one percent when $\bar{x}_1 < x < \bar{x}_2$. By (II.20), $|x_i - x_c| < \sqrt{2}/10 |\bar{x}_i - x_c|$ whenever $|\mathscr{E}(\Omega) - \mathscr{E}| < (c^3 \bar{c}^{-2} 10^{-6})\, \Omega^{-1}$.

We break the integral in (II.21) into two parts

$$\int_{x_0}^{x_1 - \varepsilon_1} = \int_{x_0}^{\bar{x}_1} + \int_{\bar{x}_1}^{x_1 - \varepsilon_1}.$$

By (II.20), $p(x) > (\text{small constant})\, \Omega^{-1}$ for $x < \bar{x}_1$. Hence, (II.19) implies

$$\begin{aligned} &\int_{x_0}^{\bar{x}_1} (|p'|^2\, |p|^{-5/2} + |p''|\, |p|^{-3/2}) \\ &\qquad < |x_0 - \bar{x}_1| \text{ const.} \cdot \Omega^{-3/2} \\ &\qquad < \text{const.} \cdot \Omega^{-1/2}. \end{aligned}$$

As (II.22) holds within 1/10 of one percent for $x \in [\bar{x}_1, \bar{x}_2]$,

$$p(x) > (\mathscr{E} - \mathscr{E}(\Omega)) + 1/2c(\Omega)\, \Omega^{-3}(x - x_c)^2\, 999/1000.$$

Since $p'(x) < c(\Omega)\,\Omega^{-3}(x-x_c)\,999/1000$ and $p''(x) < \bar{c}\Omega^{-3}$,

$$\int_{\bar{x}_1}^{x_1-\varepsilon_1} \leqslant \text{const.} \int_{\bar{x}_1}^{x_1-\varepsilon_1} \frac{\Omega^{-3}(x-x_c)^2}{[(\mathscr{E}-\mathscr{E}(\Omega))+1/2c(\Omega)\,\Omega^{-3}(x-x_c)^2\,999/1000]^{5/2}}$$

$$+\text{const.} \int_{\bar{x}_1}^{x_1-\varepsilon_1} \frac{\Omega^{-3}}{[(\mathscr{E}-\mathscr{E}(\Omega))+1/2c(\Omega)\,\Omega^{-3}(x-x_c)^2\,999/1000]^{3/2}}.$$

Change variables to $u=(2(\mathscr{E}(\Omega)-\mathscr{E})\,c(\Omega)^{-1}\Omega^3)^{-1/2}\,(x-x_c)$. The integrals are bounded by

$$\text{const.}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}\,\Omega^{-3/2}\int_{101/100}^{\infty} \frac{u^2}{[999/1000\,u^2-1]^{5/2}}\,du$$

$$+\text{const.}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}\,\Omega^{-3/2}\int_{101/100}^{\infty} \frac{1}{[999/1000\,u^2-1]^{3/2}}\,du.$$

We can analyze the supremum of (II.21) in an analogous fashion. First notice that

$$|p|^{-1/4}\left|\frac{d}{dx}|p|^{-1/4}\right| = 1/4|p|^{-3/2}\,|p'(x)|.$$

When $x<\bar{x}$, $p(x) > (\text{small constant})\cdot\Omega^{-1}$ and $|p'| < \bar{c}\,\Omega^{-2}$. Hence,

$$|p|^{-3/2}\,|p'(x)| < \text{const.}\,\Omega^{-1/2}.$$

When $x \in [\bar{x}_1, x_1-\varepsilon_1]$,

$$|p'|\,|p|^{-3/2} \leqslant \frac{\text{const.}\,\Omega^{-3}|x-x_c|}{[(\mathscr{E}-\mathscr{E}(\Omega))+1/2c(\Omega)\,\Omega^{-3}(x-x_c)^2\,999/1000]^{3/2}}$$

$$\leqslant \frac{\text{const.}\,\Omega^{3/2}|x-x_c|}{[999/1000(x-x_c)^2-2(\mathscr{E}(\Omega)-\mathscr{E})\,\Omega^3 c(\Omega)^{-1}]^{3/2}}.$$

$|x-x_c|$ ranges between $101/100\sqrt{2(\mathscr{E}(\Omega)-\mathscr{E})\,\Omega^3 c(\Omega)^{-1}}$ at $x_1-\varepsilon_1$ and const.$\cdot\,\Omega$ at $\bar{x}_1$. A simple maximization shows that the maximum value is attained at $x_1-\varepsilon_1$, where it equals

$$\text{const.}\,\Omega^{-3/2}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}.$$

Hence, we see that for $|\mathscr{E}-\mathscr{E}(\Omega)| < (c^3\bar{c}^{-2}10^{-6})\,\Omega^{-1}$, Lemma 1 can be used to approximate solutions to (II.1) on $[x_0, x_1-\varepsilon_1|$ whenever

$$Z^{1/3} > (\text{large constant})\cdot\Omega^{-3/2}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}.$$

Our aim is to prove Estimate 1 of Section 1. With this in mind, let us write this large constant as $M/100$. This determines how large M must be.

Before calculating the boundary condition at $x_1-\varepsilon_1$, let us calculate (II.21) when $|\mathscr{E}(\Omega)-\mathscr{E}|>(c^3\bar{c}^{-2}10^{-6})\,\Omega^{-1}$. In this case, the turning points are at least a small constant times Ω to the left and right of x_c. The derivative at the left turning point is at least a small multiple of Ω^{-2}. In this case, we can pick ε_1 to be another small multiple of Ω and still have it satisfy the assumptions of Lemma 3. This is obvious from the above comments and (II.19). This implies

$$\begin{aligned}\int_{x_0}^{x_1-\varepsilon_1} &(|p'|^2\,|p|^{-5/2}+|p''|\,|p|^{-3/2})\\ &<|x_0-(x_1-\varepsilon_1)|\cdot\text{const.}\cdot\Omega^{-3/2}\\ &<\text{const.}\cdot\Omega^{-1/2}.\end{aligned}$$

Similarly, $|p|^{-3/2}\,|p'|<\text{const.}\cdot\Omega^{1/2}$. Since $|\mathscr{E}(\Omega)-\mathscr{E}|>\text{const.}\cdot\Omega^{-1}$ in this case, we can absorb this in

$$(M/100)\cdot\Omega^{-3/2}\,(\mathscr{E}(\Omega)-\mathscr{E})^{-1}.$$

Let us now use Lemma 1 to establish the boundary condition for w_0 at $x_1-\varepsilon_1$. Let $Z^{1/3}>M\cdot\Omega^{-3/2}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}$. Let u_1 and u_2 be the solutions of (II.1) that Lemma 1 describes. Our solution w_0 can be written

$$w_0(x)=\alpha u_1(x)+\beta u_2(x).$$

The boundary condition (II.17) at x_0 determines α and β:

$$\alpha\begin{pmatrix}u_1\\ u_1'\end{pmatrix}(x_0)+\beta\begin{pmatrix}u_2\\ u_3'\end{pmatrix}(x_0)=\begin{pmatrix}\text{non-zero}\\ \text{constant}\end{pmatrix}\begin{pmatrix}1\\ \alpha_0\end{pmatrix}.$$

with $\alpha_0>(9/10)\,Z^{1/3}\Omega^{-1/2}$.

By Lemma 1,

$$\begin{pmatrix}u_1\\ u_1'\end{pmatrix}(x_0)=\begin{pmatrix}p^{-1/4}\\ \dfrac{d}{dx}p^{-1/4}+Z^{1/3}p^{1/4}\end{pmatrix}(x_0)+\begin{pmatrix}\varepsilon_1\\ \varepsilon_1\end{pmatrix}(x_0)$$

$$\begin{pmatrix}u_2\\ u_2'\end{pmatrix}(x_0)=\begin{pmatrix}p^{-1/4}\\ \dfrac{d}{dx}p^{-1/4}-Z^{1/3}p^{1/4}\end{pmatrix}(x_0)+\begin{pmatrix}\varepsilon_2\\ \varepsilon_1\end{pmatrix}(x_0),$$

where $(|\varepsilon_i| + |\varepsilon_i'|) < Z^{-1/3}M/20\,\Omega^{-3/2}(\mathscr{E}(\Omega) - \mathscr{E})^{-1}\,(|u_i| + |u_i'|)$. Since $0 < y(x) < 1$,

$$90\Omega^{-1} + \mathscr{E} < p(\Omega/10) < 100\Omega^{-1} + \mathscr{E}.$$

Since $\mathscr{E} < \mathscr{E}(\Omega) < (4\Omega)^{-1}$, $p(\Omega/10)$ is between $90\Omega^{-1}$ and $100\Omega^{-1}$ within a percent. Also,

$$Z^{1/3} > 2\left|p^{1/4}\frac{d}{dx}p^{-1/4}\right|.$$

Hence, we see easily that any solution to (II.22) must have $|\beta| < 2|\alpha|$. For convenience, pick $\alpha = 1$. That is, on $[x_0, x_1 - \varepsilon_1]$

$$w_0(x) = (\bar{u}_1(x) + \varepsilon_1(x)) + \beta(\bar{u}_2(x) + \varepsilon_2(x))$$

with $|\beta| < 2$. By Lemma 1, our calculation of (II.21), and our choice of $Z^{1/3}$,

$$\begin{aligned}&(|\varepsilon_1 + \beta\bar{u}_2 + \beta\varepsilon_2| + |\varepsilon_1' + \beta\bar{u}_2' + \beta\varepsilon_2'|)(x_1 - \varepsilon_1)\\ &\quad < \left(1/20 + 2\exp\left[-2Z^{1/3}\int_{x_0}^{x_1-\varepsilon_1} p^{1/2}(t)\,dt\right]\right)(|\bar{u}_1| + |\bar{u}_1'|)(x_1 - \varepsilon_1).\end{aligned} \tag{II.23}$$

Since $\Omega x^{-2} - y(x)\,x^{-1} > \Omega x^{-2} - x^{-1}$, $x_1 > \Omega$. Furthermore, $\Omega x^{-2} - y(x)\,x^{-1} > 2\Omega^{-1}$ when $x < \Omega/2$. Hence,

$$\int_{x_0}^{x_1-\varepsilon_1} p^{1/2}(t)\,dt > (\Omega/2 - \Omega/10)\cdot\sqrt{2}\,\Omega^{-1/2} > 1/2\Omega^{-1/2}.$$

Since $\Omega > \Omega(Z) = (L(Z)+1)L(Z)\,Z^{-2/3} \approx Z^{2/9-2/3}$, we see that

$$2\exp\left[-2Z^{1/3}\int_{x_0}^{x_1-\varepsilon_1} p(t)\,dt\right] \ll 1$$

for large Z. Coupling this with (II.23), we see

$$(|w_0 - \bar{u}_1| + |w_0' - \bar{u}_1'|)(x_1 - \varepsilon_1) < (1/10)(|\bar{u}_1| + |\bar{u}_1'|)(x_1 - \varepsilon_1). \tag{II.24}$$

We can use Lemma 3 to extend w_0 across $[x_1 - \varepsilon_1, x_1 + \varepsilon_1]$. First, let us calculate the approximation error

$$C = \varepsilon_1^{-3/2}\,p'(x_1)^{-1/2}$$

of Lemma 3. When $|\mathscr{E}(\Omega)-\mathscr{E}|<(c^2\bar{c}^{-2}10^{-6})\,\Omega^{-1}$, (II.20) shows that

$$C=\text{const.}\,\Omega^{-3/2}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}.$$

When $|\mathscr{E}(\Omega)-\mathscr{E}|>(c^3\bar{c}^{-2}10^{-6})\,\Omega^{-1}$, we have noted that

$$p'(x_1)>\text{const.}\,\Omega^{-2}$$

$$\varepsilon_1>\text{const.}\,\Omega.$$

Hence $C=\text{const.}\,\Omega^{-1/2}$ in this case. In Lemma 3, C is multiplied by a constant $\tilde{K}$ arising in the uniform approximation by Airy functions. Let us increase the constant γ appearing in the statement of Estimate 1 of Section 0 enough to imply

$$KC<M/100\,\Omega^{-3/2}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}.$$

Our assumption

$$Z^{1/3}>M\Omega^{-3/2}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}$$

satisfies the conditions necessary to apply Lemma 3 on $[x_1-\varepsilon_1, x_1+\varepsilon_1]$.

Again, we must find the α and β which solve

$$\begin{pmatrix} w_0 \\ w_1' \end{pmatrix}(x_1-\varepsilon_1)=\left[\alpha\begin{pmatrix} w_1 \\ w_1' \end{pmatrix}+\beta\begin{pmatrix} w_2 \\ w_2' \end{pmatrix}\right](x_1-\varepsilon_1), \tag{II.25}$$

where w_1 and w_2 are the solutions of (II.1) described by Lemma 3. The approximation $\bar{w}_i$ in Lemma 3 and the $\bar{u}_i$ in Lemma 1 are related by

$$\begin{aligned} \bar{w}_1(x)&=\exp\left[-Z^{1/3}\int_{x_0}^{x_1}p^{1/2}(t)\,dt\right]\bar{u}_1(x)\\ \bar{w}_2(x)&=\exp\left[Z^{1/3}\int_{x_0}^{x_1}p^{1/2}(t)\,dt\right]\bar{u}_2(x). \end{aligned} \tag{II.26}$$

By (II.24) and (II.25), we must have

$$\begin{aligned} &(|\alpha w_1+\beta w_2-\bar{u}_1|+|\alpha w_1'+w_2'-\bar{u}_1'|)(x_1-\varepsilon_1)\\ &\quad<(1/10)(|\bar{u}_1|+|\bar{u}_1'|)(x_1-\varepsilon_1). \end{aligned} \tag{II.27}$$

By Lemma 3,

$$\begin{aligned} &(|\alpha w_1+w_2-\bar{u}_1|+|\alpha w_1'+\beta w_2'-\bar{u}_1'|)(x_1-\varepsilon_1)\\ &\quad\geqslant(|\alpha\bar{w}_1+\beta\bar{w}_2-\bar{u}_1)|+|\alpha\bar{w}_1'+\beta\bar{w}_2'-\bar{u}_1'|)(x_1-\varepsilon_1)\\ &\qquad-\tilde{K}\cdot C\cdot Z^{-1/3}[\alpha(|\bar{w}_1|+|\bar{w}'|)+\beta(|\bar{w}_2|+|\bar{w}_2'|)]. \end{aligned} \tag{II.28}$$

By assumptions, $\tilde{K} \cdot C \cdot Z^{-1/3} \ll 1$. By (II.26) and the definition of $\bar{u}_i$, we see that

$$|\bar{w}_2|(x_1 - \varepsilon_1) > \exp\left[Z^{1/3} \int_{x_1-\varepsilon_1}^{x_1} p^{1/2}\right] \cdot \exp\left[-Z^{1/3} \int_{x_0}^{x_1-\varepsilon_1} p^{1/2}\right] |\bar{u}_1|$$

$$|w_2'|(x_1 - \varepsilon_1) > \exp\left[Z^{1/3} \int_{x_1-\varepsilon_1}^{x_1} p^{1/2}\right] \cdot \exp\left[-Z^{1/3} \int_{x_0}^{x_1-\varepsilon_1} p^{1/2}\right] |\bar{u}_1'|.$$

By (II.28), we see that (II.27) can hold only if

$$\beta \exp\left[Z^{1/3} \int_{x_1-\varepsilon_1}^{x_1} p^{1/2}\right] \cdot \exp\left[-Z^{1/3} \int_{x_0}^{x_1-\varepsilon_1} p^{1/2}\right] < 2.$$

On the other hand,

$$\beta \bar{w}_2' - \bar{u}_1' < -\frac{1}{2} Z^{1/3} p^{1/4} \bar{u}_1, \qquad 0 < \bar{w}_1' < \exp\left[-Z^{1/3} \int_{x_0}^{x_1} p^{1/2}\right] Z^{1/3} p^{1/4} \bar{u}_1,$$

and $|\bar{u}_1'| < Z^{1/3} p^{1/4} |\bar{u}_1|$.

Since $Z^{1/3} p^{1/4} (x_1 - \varepsilon_1) \gg 1$, (II.27) and (II.28) can hold only if

$$\alpha > \frac{1}{4} \exp\left[Z^{1/3} \int_{x_0}^{x_1} p^{1/2}\right].$$

By linear independence of w_1 and w_2, we know a solution to (II.25) exists. We have just shown that

$$2 > \frac{1}{4} \exp\left[2Z^{1/3} \int_{x_1-\varepsilon_1}^{x_1} p^{1/2}(t)\, dt\right].$$

By our choice of ε_1,

$$\int_{x_1-\varepsilon_1}^{x_1} p^{1/2}(t)\, dt = 2p'(x_1)^{1/2}\, \varepsilon_1^{3/2}$$

within a factor which is close to 1. As we have noted,

$$\tilde{K} \cdot p^{-1/2} \varepsilon_1^{-3/2} < M/100\, \Omega^{-3/2} (\mathscr{E}(\Omega) - \mathscr{E})^{-1}.$$

Let us renormalize, taking $\alpha = 1$. We have proved

$$w_0(x) = w_1(x) + \beta w_2(x)$$

on $[x_1 - \varepsilon_1, x_1 + \varepsilon_1]$, with

$$\beta < K/25\, Z^{-1/3} \Omega^{-3/2} (\mathscr{E}(\Omega) - \mathscr{E})^{-1}.$$

By our choice of $Z^{1/3}$, $\beta \ll 1$. Lemma 3 implies that the phase of w_0 at $x_1+\varepsilon_1$ is given by

$$\begin{pmatrix} w_0 \\ w_0' \end{pmatrix}(x_1+\varepsilon_1)=\left[c_1\begin{pmatrix} \bar{w}_1 \\ \bar{w}' \end{pmatrix}+c_2\begin{pmatrix} \bar{w}_2 \\ \bar{w}_2' \end{pmatrix}\right](x_1+\varepsilon_1) \tag{II.29}$$

with

$$|c_1-1|<Z^{-1/3}\,M/10\Omega^{-3/2}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}$$
$$|c_2|<Z^{-1/3}\,M/10\Omega^{-3/2}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}.$$

We can use Lemma 2 and (II.29) to extend w_0 across the interval $[x_1+\varepsilon_1, x_2-\varepsilon_2]$. To do so, we must first calculate ε_2 and then the approximation errors in Lemma 2.

We have already calculated the right turning when $|\mathscr{E}-\mathscr{E}(\Omega)|<(c^3\bar{c}^{-2}10^{-6})\,\Omega^{-1}$—that is, when the quadratic approximation is useful for calculations. See (II.20). Within 1/10 of one percent,

$$\begin{aligned} x_2-x_c&=\sqrt{2(\mathscr{E}(\Omega)-\mathscr{E})\,c(\Omega)^{-1}\,\Omega^3} \\ p'(x)&=C(\Omega)\,\Omega^{-3}(x-x_2) \qquad \text{for all} \quad |x-x_2|<2|x_1-x_c|. \end{aligned} \tag{II.30}$$

For Lemma 2 to apply, $Z^{-1/3}$ must be large compared to

$$\int_{x_1+\varepsilon_1}^{x_2-\varepsilon_2}(|p'|^2\,|p|^{-5/2}+|p''|\,|p|^{-3/2})$$
$$\sup\left\{|p|^{-1/4}\left|\frac{d}{dx}|p|^{-1/4}\right|\,\middle|\,x_1+\varepsilon_1<x<x_2-\varepsilon_2\right\}. \tag{II.31}$$

By (II.30) $|p'|$ takes its maximum and $|p|$ its minimum at the endpoints of the interval. Since $|p''|<\bar{c}\Omega^{-3}$, we find that both quantities in (II.31) are bounded by

$$\text{const.}\ \Omega^{-3/2}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}.$$

By possibly increasing the M we have been using in all our estimates, this is

$$<M/100\,\Omega^{-3/2}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}.$$

Since $Z^{1/3}>M\Omega^{-3/2}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}$, Lemma 2 applies.

When $\mathscr{E}$ decreases out of the range $|\mathscr{E}-\mathscr{E}(\Omega)|<(c^3\bar{c}^{-2}10^{-6})\,\Omega^{-1}$, the left turning point x_1 moves between a small multiple of Ω to the left of $x_c(\Omega)$, toward Ω. It always lies between Ω and $x_c(\Omega)$. The right turning point x_2 changes much more. We take several special cases. Let $\bar{x}$ be a number so large that $y(x)$ and its first three derivatives equal $144x^{-3}$ and its first three derivatives within one percent error for all $x > \bar{x}$. We classify $\mathscr{E}$ accordingly as

(a) $x_2 \in [x_c(\Omega) + \text{const.}\ \Omega, 2\bar{x}]$,

(b) $x_2 > 2\bar{x}$.

The "const." in (a) is determined by the condition that $x_2 = x_c(\Omega) + \text{const.}\ \Omega$ when $\mathscr{E} = \mathscr{E}(\Omega) - (c^3\bar{c}^{-2}10^{-6})^{-1}$. Notice that depending on $\Omega < \bar{\Omega}$, (a) or both (a) and (b) might be empty. In case (a), we can use the bounds

$$\begin{aligned}(\text{small const.})\, x^{-2} < p'(x) &< x^{-2}\\ |p''(x)| &< \text{const.}\ x^{-3}\\ |p'''(x)| &< \text{const.}\ x^{-4}.\end{aligned} \tag{II.32}$$

These constants are uniform in Ω for $x_c(\Omega) + \text{const.}\ \Omega < x < \min\{2\bar{x}, x_\infty(\Omega)\}$. To see this, note that if Ω is large enough that $x_\infty(\Omega) = (x_2(\Omega) + x_m(\Omega))/2 < 2\bar{x}$, then Corollary 2 gives uniform bounds which imply the ones we have written above. On the other hand, if Ω is small enough that $(x_2(\Omega) + x_m(\Omega))/2 > 2\bar{x}$ then we know that $[2\Omega + \text{const.}\ \Omega, 2\bar{x}]$ is strictly contained in the range where $p(x)$ is increasing. We have

$$p'(x) = -2\Omega x^{-3} + (y(x) - xy'(x))\, x^{-2}.$$

The function $y(x) - xy'(x)$ is strictly positive. By explicit calculation using the series expansion for $y(x)$ in the regime $[\Omega, 1/100]$, we know that

$$(-2\Omega x^{-1} + y(x) - xy'(x))$$

is greater than a small constant once $x \in [2\Omega + \text{const.}\ \Omega, 1/100]$. Let Ω_0 be such that

$$(x_2(\Omega_0) + x_m(\Omega_0))/2 = 2\bar{x}.$$

Since $-2\Omega_0 x^{-1} + (y(x) - xy'(x)) > \text{constant}$ for $x \in [1/100, 2\bar{x}]$, we see that the same bound holds for all smaller Ω.

From (II.32), we see that once ε_2 is a suitably small multiple of x_2, it satisfies the assumptions of Lemma 3. Furthermore, the error

$$C \equiv p(x_2)^{-1/2}\, \varepsilon_2^{-3/2} < (\text{large constant})\, x_2^{-1/2}, \tag{II.33}$$

when $x_2 < 2x$.

To calculate (II.31) in this case, we break the integral into two pieces:

$$\int_{x_1+\varepsilon_1}^{x_2-\varepsilon_1} = \int_{x_1+\varepsilon_1}^{2\Omega} + \int_{2\Omega}^{x_2-\varepsilon_2}.$$

Using (II.19) and our choice of ε_1 as a small multiple of Ω, we bound the first integral by

$$\text{const. } \Omega^{-1/2}.$$

To bound the second integral, notice that $|p(x)| = |\int_x^{x_2} p'(x)|$. By (II.32) and our choice of ε_2 as a small constant times x_2, we find

$$|p| > (\text{small const.}) \cdot x^{-1}$$

when $2\Omega < x < x_2 - \varepsilon_2$. Equation (II.32) then implies

$$\begin{aligned} &\int_{2\Omega}^{x_2 - \varepsilon_2} (|p'|^2 \, |p|^{-5/2} + |p''| \, |p|^{-3/2}) \, dx \\ &\quad < \text{const.} \int_{2\Omega}^{x_2} x^{-3/2} \, dx \\ &\quad < \text{const. } \Omega^{-1/2}. \end{aligned}$$

The supremum in (II.31) is calculated via the same bounds—i.e., (II.19) for $x < 2\Omega$ and (II.31) for $x > 2\Omega$. It is also less than const. $\Omega^{1/2}$. Hence,

$$\text{(II.31) is } < \text{ const. } \Omega^{-1/2}$$

in case (a).

In case (b), we break the integral as

$$\int_{x_1 + \varepsilon_1}^{x_2 - a_1} = \int_{x_1 + \varepsilon_1}^{\bar{x}} + \int_{\bar{x}}^{x_2 - \varepsilon_2}.$$

The first integral and the supremum over $x \in [x_1 + \varepsilon_1, \bar{x}]$ is handled as in case (a) yielding const. $\Omega^{-1/2}$. For $x > \bar{x}$ we use the fact that $y(x) \sim 144x^{-3}$ in this region. First, let us calculate $x_2(\Omega)$ and $x_m(\Omega)$. $x_2(\Omega)$ solves

$$\Omega x^{-2} - 144x^{-4} = 0,$$

and $x_m(\Omega)$ solves

$$-2\Omega x^{-3} + 4 \cdot 144x^{-5} = 0.$$

Within a small percentage error

$$x_2(\Omega) = 12\Omega^{-1/2}$$

and

$$x_m(\Omega) = \sqrt{2} \cdot 12\Omega^{-1/2}.$$

By inspection, we see that for $x \in [\bar{x}, x_\infty(\Omega)]$

$$\begin{aligned}(\text{smaller const.})\, x^{-5} < p'(x) &< \text{const. } x^{-5}\\ |p''(x)| &< \text{const. } x^{-6} \qquad \text{(II.34)}\\ |p'''(x)| &< \text{const. } x^{-7}.\end{aligned}$$

Again, we can pick ε_2 to be a small multiple of x_2. The error C in Lemma 3 is

$$C \equiv p'(x_2)^{-1/2}\, \varepsilon_2^{-3/2} \leqslant \text{const. } x_2 \leqslant \text{const. } \Omega^{-1/2}. \qquad \text{(II.35)}$$

Using (II.34) and our choice of ε_2, we find

$$|p(x)| = \left|\int_x^{x_2} p'(x)\right| > \text{const. } x^{-4} \qquad \text{for} \quad x \in [\bar{x}, x_2 - \varepsilon_2].$$

Hence,

$$\begin{aligned}&\int_{\bar{x}}^{x_2-\varepsilon_2} (|p'|^2\, |p|^{-5/2} + |p''|\, |p|^{-3/2})\\ &\qquad \leqslant \text{const. } \int_x^{x_2} dx \leqslant \text{const. } x_2 \leqslant \text{const.} \cdot \Omega^{-1/2}.\end{aligned}$$

The supremum in (II.31) satisfies the same estimate.

Again, we increase the constant M that we have used throughout this analysis so that we have

$$\text{(II.31) is } < M/100\Omega^{-3/2}(\mathscr{E}(\Omega) - \mathscr{E})^{-1}.$$

Since $Z^{1/3} > M\Omega^{-3/2}(\mathscr{E}(\Omega) - \mathscr{E})^{-1}$, we can use Lemma 2 to extend w_0' across $[x_1 + \varepsilon_1, x_2 - \varepsilon_2]$. Let v_1 and v_2 be the two solutions to (II.1) which are described in Lemma 2. Again, we must find α and β for which

$$\begin{pmatrix} w_0 \\ w_0' \end{pmatrix} (x_1 + \varepsilon_1) = \alpha \begin{pmatrix} v_1 \\ v_1' \end{pmatrix} (x_1 + \varepsilon_1) + \beta \begin{pmatrix} v_2 \\ v_2' \end{pmatrix} (x_1 + \varepsilon_1).$$

By Lemma 2 this equals

$$\bar{\alpha} \begin{pmatrix} \bar{v}_1 \\ \bar{v}_1' \end{pmatrix} (x_1 + \varepsilon_1) + \bar{\beta} \begin{pmatrix} \bar{v}_2 \\ \bar{v}_2' \end{pmatrix} (x_1 + \varepsilon_1),$$

where $|\bar{\alpha} - \alpha| + |\bar{\beta} - \beta| < Z^{-1/3}\gamma/20\, \bar{\Omega}^{3/2}(\mathscr{E}(\Omega) - \mathscr{E})^{-1}\, (|\alpha| + |\beta|)$. In Lemma 2, we choose linearly independent solutions to (II.1) that are approximated by $\bar{v}_1 = |p|^{-1/4} \cos[\int_{x_1+\varepsilon_1}^{x} |p|^{1/2}]$ and $\bar{v}_2 = |p|^{-1/4} \sin[\int_{x_1+\varepsilon_1}^{x} |p|^{1/2}]$. By taking a linear combination we can assume

$$\bar{v}_1 = |p|^{-1/4} \cos\left[Z^{1/3} \int_c^x |p|^{1/2} - \pi/4 \right]$$

$$\bar{v}_2 = |p|^{-1/4} \cos\left[Z^{1/3} \int_c^x |p|^{1/2} + \pi/4 \right].$$

By (II.29), we see that $|\bar{\alpha} - 1|$ and $|\bar{\beta}|$ are both less than $Z^{-1/3} M/10\Omega^{-3/2}(\mathscr{E}(\Omega) - \mathscr{E})^{-1}$. Hence, the same holds for α and β, with the "10" replaced by a "5."

This implies a boundary condition for w_0 at $x_2 - \varepsilon_2$:

$$\begin{pmatrix} w \\ w_0' \end{pmatrix} (x_2 - \varepsilon_2) = c_1 \begin{pmatrix} \bar{v}_1 \\ \bar{v}_1' \end{pmatrix} (x_2 - \varepsilon_2) + c_2 \begin{pmatrix} \bar{v}_2 \\ \bar{v}_2' \end{pmatrix} (x_2 - \varepsilon_2) \qquad \text{(II.36)}$$

with $|c_1 - 1|$ and $|c_2|$ both less than $Z^{-1/3} M/5\Omega^{-3/2}(\mathscr{E}(\Omega) - \mathscr{E})^{-1}$.

By means of Lemmas 1 and 3 we can extend the solution w which satisfies (II.18) at $x = x_\infty$. We have already seen from our quadratic approximation, (II.33), and (II.35) that the approximation error from Lemma 3 on $[x_2 - \varepsilon_2, x_2 + \varepsilon_2]$ is bounded by $Z^{-1/3} M/100\Omega^{-3/2}$ $(\mathscr{E}(\Omega) - \mathscr{E})^{-1}$. By the same arguments as with w_0, we will have

$$\begin{pmatrix} w_\infty \\ w_\infty' \end{pmatrix} (x_2 - \varepsilon_2) = a + \begin{pmatrix} \bar{w}_2 \\ w_1' \end{pmatrix} + a_2 \begin{pmatrix} \bar{w}_2 \\ w_2' \end{pmatrix} (x_2 - \varepsilon_2) \qquad \text{(II.37)}$$

with $|a_1 - 1|$ and $|a_2| < Z^{-1/3}(K/5)\, \Omega^{-3/2}(\mathscr{E}(\Omega) - \mathscr{E})^{-1}$ and

$$\bar{w}_1 = |p|^{-1/4} \cos\left[Z^{1/3} \int_x^{x_2} |p|^{1/2}\, dt - \pi/4 \right]$$

$$\bar{w}_2 = |p|^{-1/4} \cos\left[Z^{1/3} \int_x^{x_2} |p|^{1/2}\, dt + \pi/4 \right],$$

once we prove that the conditions of Lemma 1 hold. We must check that $Z^{1/3}$ is large compared to

$$\int_{x_2+\varepsilon_2}^{x} (|p'|^2\, |p|^{-5/2} + |p''|\, |p|^{-3/2}$$

$$\sup\left\{ |p|^{-1/4} \left| \frac{d}{dx} |p|^{-1/4} \right| \,\middle|\, x_2 + \varepsilon_2 < x < x_\infty \right\}. \qquad \text{(II.38)}$$

We prove that (II.38) is small compared to $M\Omega^{-3/2}(\mathscr{E}(\Omega) - \mathscr{E})^{-1}$.

When $(\mathscr{E}-\mathscr{E}(\Omega))<(c^3\bar{c}^{-2}10^{-6})\,\Omega^{-1}$, the second turning point x_2 is given by (II.20). Define $\bar{x}_2=x_c+10^{-3}c c^{-1}\Omega$. By (II.20), $|x_2-x_c|<\sqrt{2}|\bar{x}_2-x_c|$ when $|\mathscr{E}(\Omega)-\mathscr{E}|<(c^3\bar{c}^{-2}10^{-6})\,\Omega^{-1}$. We break the quantities in (II.38) into two parts:

$$\int_{x_2+\varepsilon_2}^{x}=\int_{x_2+\varepsilon_2}^{\bar{x}_2}+\int_{\bar{x}_2}^{x}.$$

The analysis of the first integral follows that for the analogous integral in (II.21). There, we found it was bounded by

$$M/100\,\Omega^{-3/2}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}.$$

For the second integral (II.32) and (when Ω is small) (II.34) are appropriate. By (II.32) and the fact that $\bar{x}_2>x_2+\text{const.}\,\Omega$, $|p(x)|>\text{const.}\,x^{-1}$ when $x<\bar{x}$. We have

$$\int_{\bar{x}_2}^{\bar{x}}(|p'|^2\,|p|^{-5/2}+|p''|\,|p|^{-3/2})$$

$$<\text{const.}\int_{\bar{x}_2}^{\bar{x}}x^{-3/2}\,dx$$

$$<\text{const.}\,\bar{x}_2^{-1/2}<\text{const.}\,\Omega^{-1/2}.$$

Since $x_\infty(\Omega)<\text{const.}\,\Omega^{-1/2}$ and the integrand is uniformly bounded for $x>\bar{x}$, we have proved that

$$\text{(II.38) is }<M/100\,\Omega^{-3/2}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}$$

in this case.

When $x_c+\text{const.}\,\Omega<x_2<\bar{x}$, we use (II.32) and (II.34) as we did for the second integral above. That is, since $\varepsilon_2>\text{const.}\,x_2$, (II.32) implies that $|p(x)|>\text{const.}\,x^{-1}$ for $x_2+\varepsilon_2<x<2\bar{x}$. When $x>2\bar{x}$, the integrand is uniformly bounded. In this case, we obtain the bound

$$<\text{const.}\,\Omega^{-1/2}.$$

When $x_2>\bar{x}$, we use (II.34). Since $\varepsilon_2>\text{const.}\,x_2$, $|p(x)|>\text{const.}\,x^{-4}$ once $x>x_2+\varepsilon_2$. By (II.34),

$$\int_{x_2+\varepsilon_2}^{x}(|p'|^2\,|p|^{-5/2}+|p''|\,|p|^{-3/2})$$

$$<\int_{x_2}^{x}\text{const.}<\text{const.}\,\Omega^{-1/2}.$$

The same bounds imply these estimates for the supremum also. Possibly increasing M, this proves

$$(\text{II.38}) < M/100\, \Omega^{-3/2}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}$$

in all cases.

Let us now examine the implications of (II.36) and (II.37). For $\mathscr{E}$ to be an eigenvalue, the two vectors must be non-zero multiples of each other. To normalize, assume $c_1^2+c_2^2=1$, $a_1^2+a_2^2=1$. Write $c_1=\cos\delta_0$, $c_2=-\sin\delta_0$, $a_1=\cos\delta_\infty$, $a_2=-\sin\delta_\infty$. By (II.36) and (II.37), $|\delta_0|$ and $|\delta_\infty|$ are each less than

$$Z^{-1/3}\, M/5\, \Omega^{-3/2}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}.$$

Writing out (II.36) and (II.37), we see that

$$\begin{aligned}&\begin{pmatrix}\cos\\ \sin\end{pmatrix}\left(Z^{1/3}\int_{x_1}^{x_2-\varepsilon_2}|p|-\pi/4+\delta_0\right)\\ &\quad=\pm\begin{pmatrix}\cos\\ -\sin\end{pmatrix}\left(Z^{1/3}\int_{x_2-\varepsilon_2}^{x_2}|p|^{1/2}-\pi/4+\delta_\infty\right).\end{aligned}\tag{II.39}$$

This implies that the sum of the two arguments equals zero mod π. That is,

$$Z^{1/3}\int_{x_1}^{x_2}|p|^{1/2}(t)\,dt-\pi/2+\delta_0+\delta_\infty=n\pi.$$

Since $|\delta_0|, |\delta_\infty| \ll 1$, this implies that

$$Z^{1/3}\int_{x_1}^{x_2}|p|^{1/2}(t)\,dt=\pi/2+n\pi-\delta_0-\delta_\infty\tag{II.40}$$

for some non-negative integer n and δ_0 and δ_∞ satisfying

$$|\delta_0|, |\delta_\infty| < Z^{-1/3}(M/5)\,\Omega^{3/2}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}.$$

For us, $p(x)=[\Omega x^{-1/2}-y(x)\,x^{-1}+\mathscr{E}]$. Notice that we could just as easily have obtained (II.40) by equating the phases of w_0 and w_∞ at $x=x_c(\Omega)$. As $\mathscr{E}$ decreases from $\mathscr{E}(\Omega)$, the phase of w_0 at x_c strictly increases in a clockwise direction around the unit circle and the phase of w_∞ at x_c strictly decreases in a counterclockwise direction. An eigenvalue $\mathscr{E}_k$ is a value of $\mathscr{E}$ for which the two agree modulo parity. Equations (II.36) and (II.37) with x_c replacing $x_2-\varepsilon_2$ allow us to compute these phases within a small error and see that each makes half a rotation around the unit circle for each increase in $Z^{1/3}\int_{x_1}^{x_2}|p|^{1/2}\,dt$ by π. This implies one new eigenvalue $\mathscr{E}_k$ for each increase in $Z^{1/3}\int_{x_1}^{x_2}|p|^{1/2}\,dt$ by π.

Once again, let

$$K(Z,\Omega)=\min\{k\,|\,\mathscr{E}_k<\mathscr{E}(\Omega)-10M\,\Omega^{-3/2}Z^{-1/3}\}.$$

In view of the above discussion, (II.40) implies

$$(Z^{1/3}/\pi)\int_{x_1}^{x_2}|y(\gamma^{-1}x)\,x^{-1}-\Omega x^{-2}-\mathscr{E}_k|^{1/2}\,dx$$
$$=k+\frac{1}{2}+\delta(Z,\Omega,\mathscr{E}_k)+\tilde{k}(Z,\Omega)$$

for $k\geqslant K(Z,\Omega)$, where $\tilde{k}(Z,\Omega)$ is some integer. That is, we have proved that the eigenvalues $\mathscr{E}_{K(Z,\Omega)}>\mathscr{E}_{K(Z,\Omega)+1}>\dots$ solve the above equations for some unit increment increasing sequence of integers on the right-hand side. The WKB Theorem states that $\tilde{k}(Z,\Omega)=0$. Once we prove it, we will have established the second part of the WKB Theorem, i.e., the eigenvalue equation for $0\leqslant\mathscr{E}_k\leqslant\mathscr{E}(\Omega)-10MZ^{-1/3}\Omega^{-3/2}$.

This step is intimately connected to the WKB Theorem for $\mathscr{E}(\Omega)-10MZ^{-1/3}\Omega^{-3/2}\leqslant\mathscr{E}_k\leqslant\mathscr{E}(\Omega)$ and to Estimate 3. All hinge on the accuracy of the quadratic approximation around and between the turning points of

$$[y(\gamma^{-1}x)\,x^{-1}-\Omega x^{-2}-\mathscr{E}]$$

when $\mathscr{E}(\Omega)-10MZ^{-1/3}\mathscr{E}^{-3/2}<\mathscr{E}<\mathscr{E}(\Omega)$. This approximation allows us to estimate the eigenvalues $\mathscr{E}_k$ in terms of those for the harmonic oscillator, for which the WKB eigenvalue equation is exact.

As we have seen numerous times in the course of this analysis, the quadratic approximation is useful for calculations when $|\mathscr{E}-\mathscr{E}(\Omega)|<(c^3\bar{c}^{-2}10^{-6})\,\Omega^{-1}$. Since $\Omega>\Omega(Z)\approx Z^{-4/9}$ (see end of Section 0), $10MZ^{-1/3}\Omega^{-1/2}\ll 1$ once Z is large (independently of Ω). The $\mathscr{E}_k$ under consideration are well within the regime of good quadratic approximation.

The turning points x_1 and x_2 of $p(x)=[\Omega x^{-3}-y(x)\,x^{-1}+\mathscr{E}]$ are given within a fraction of a percent by

$$|x_i-x_c|=\sqrt{2(\mathscr{E}(\Omega)-\mathscr{E})\,p''(x_c)^{-1}}.$$

When $|\mathscr{E}-\mathscr{E}(\Omega)|<10MZ^{-1/3}\Omega^{-3/2}$,

$$|x_i-x_c|<\sqrt{20MZ^{-1/3}\Omega^{-3/2}p''(x_c)^{-1}}.$$

Define $\bar{x}_1 < x_c < \bar{x}_2$ by

$$|\bar{x}_i - x_c| = Z^{1/36}\sqrt{20MZ^{-1/3}\Omega^{-3/2}p''(x_c)^{-1}}.$$

On $[\bar{x}_1, \bar{x}_2]$, $p(x) = (1/2)\,p''(x_c)(x-x_c)^2 + \mathscr{E} - \mathscr{E}(\Omega) + g(x)$, with $|g(x)| \leqslant |p''(x_c)|\,|x-x_c|^2$. Hence,

$$p(x) \underset{(\leqslant)}{\geqslant} (1/2)\,p''(x_c)(x-x_c)^2\,(1 \underset{(+)}{-} |x-x_c|\,|p'''(x_c)|\,|p''(x_c)|^{-1}).$$

Recall $|p'''(x_c)|\,|p''(x_c)|^{-1} < \bar{c}\Omega^{-1}$, $p''(x_c) > c\Omega^{-3}$, and $Z^{-4/9} < \Omega < \bar{\Omega}$. Hence,

$$|x-x_c|\,|p'''(x_c)|\,|p''(x_c)|^{-1} \leqslant \text{const.}\,Z^{-1/36}$$

for $x \in [\bar{x}_1, \bar{x}_2]$. This implies

$$p(x) \underset{(<)}{>} K_{\underset{(+)}{-}}(x-x_c)^2 + \mathscr{E} - \mathscr{E}(\Omega)$$

on $[\bar{x}_1, x_2]$ with

$$K_{\underset{(+)}{-}} = (1/2)\,p''(x_c)(1 \underset{(+)}{-} \text{const.}\,Z^{-1/36}).$$

Define potentials V_- and V_+ by

$$V_{\underset{(+)}{-}}(x) = p(x) \qquad \text{if} \quad x \notin [\bar{x}_1, \bar{x}_2]$$

$$= K_{\underset{(+)}{-}}(x-x_c)^2 + \mathscr{E} - \mathscr{E}(\Omega) \qquad \text{if} \quad x \in [\bar{x}_1, \bar{x}_2].$$

The eigenvalues $-\mathscr{E}_k$ are bounded below and above by the corresponding eigenvalues for V_- and V_+, respectively. Call these $-\mathscr{E}_k^-$ and $-\mathscr{E}_k^+$. We have

$$\mathscr{E}_k^+ < \mathscr{E}_k < \mathscr{E}_k^-.$$

By comparison with the harmonic oscillator, we can directly compute the $\mathscr{E}_k^+$ and $\mathscr{E}_k^-$ for which the turning points are contained in $[\bar{x}_1, \bar{x}_2]$. By definition this includes all those $\mathscr{E}_k$ which lie between $-\mathscr{E}(\Omega)$ and $-\mathscr{E}(\Omega) + 10MZ^{-1/3}\Omega^{-3/2}$ (and many more). For large Z, $\mathscr{E}_k^+$ and $\mathscr{E}_k^-$ are close enough that our calculations are sharp enough to prove $\tilde{k}(Z, \Omega) = 0$ and the WKB Theorem. Estimate 3 (the fact that there is a uniformly bounded number of eigenvalues between $-\mathscr{E}(\Omega)$ and $-\mathscr{E}(\Omega) + 10MZ^{-1/3}\Omega^{-3/2}$) trivially follows.

We deal with the $\mathscr{E}_k^+$ first. The analysis for $\mathscr{E}_k^-$ is exactly similar. Let w_0 and w_∞ be solutions to

$$-w'' + Z^{2/3} V_+(x)\, w = 0, \tag{II.42}$$

where w_0 is L^2 at the origin and w_∞ is L^2 at infinity. Assume the trial $\mathscr{E}$ of (II.41) gives rise to turning points which lie within $[\bar{x}_1, \bar{x}_2]$. The boundary conditions (II.17) and (II.18) imply

$$\begin{pmatrix} w_0 \\ w_0' \end{pmatrix}(\bar{x}_1) = \begin{pmatrix} 1 \\ \alpha_1 \end{pmatrix}, \qquad \begin{pmatrix} w_\infty \\ w_\infty' \end{pmatrix}(\bar{x}_2) = \begin{pmatrix} 1 \\ -\alpha_2 \end{pmatrix},$$

where $\alpha_i = \alpha_i(Z, \Omega) > \text{const. } Z^{1/3} \Omega^{-1/2}$.

Change variables to $\xi = (x - x_c) Z^{1/6} K_+^{1/4}$. The interval $[\bar{x}_1, \bar{x}_2]$ becomes $[-\bar{\xi}, +\bar{\xi}]$ with

$$|\pm \bar{\xi}| > \text{const. } Z^{1/36}. \tag{II.43}$$

The boundary conditions at $\pm \bar{\xi}$ are

$$\begin{pmatrix} w_0 \\ w_0' \end{pmatrix}(-\bar{\xi}) = \begin{pmatrix} 1 \\ \alpha_1 \end{pmatrix}, \qquad \begin{pmatrix} w_\infty \\ w_\infty' \end{pmatrix}(\bar{\xi}) = \begin{pmatrix} 1 \\ -\alpha_2 \end{pmatrix} \tag{II.44}$$

with $\alpha_i(Z, \Omega) > \text{const. } Z^{1/6} \Omega^{-1/4}$. Since $\Omega < \bar{\Omega} < \infty$ for all Z, the α_i are uniformly bounded below by a constant multiple of $Z^{1/6}$. Equation (II.42) can be rewritten in the ξ variable as

$$w''(\xi) - (\xi^2 - \lambda)\, w(\xi) = 0, \tag{II.45}$$

where $\lambda = (\mathscr{E}(\Omega) - \mathscr{E}) Z^{1/3} K_+^{-1/2}$. Since $K_+ = 1/2p''(x_2)\ (1 + \text{const. } Z^{-1/36}) \geqslant c(\Omega)\, \Omega^{-3}$ and $(\mathscr{E}(\Omega) - \mathscr{E}) < 10 M Z^{-1/3} \Omega^{-3/2}$, $\lambda \leqslant \bar{\lambda}$, a constant which is independent of Ω and Z.

Equations (II.43)–(II.45) allow a comparison with the L^2 eigenvalue problem for the harmonic oscillator over all of $[-\infty, \infty]$. These eigenvalues are given by $\lambda_n = 2n + 1$. It is a well-known fact that

$$\pi^{-1} \int [\xi^2 - (2n+1)]_+^{1/2} = n + \frac{1}{2}. \tag{II.46}$$

That is, the WKB Theorem is exact for the harmonic oscillator. For the boundary conditions (II.44) at $\pm \bar{\xi}$ replacing that L^2 condition at $\pm \infty$, the eigenvalues λ_n^+ (corresponding to K_+) are given by

$$\lambda_n^+ = 2k + 1 + o(1) \qquad \text{as} \quad Z \to \infty,$$

uniformly for $k <$ any fixed integer K. The same, of course, holds for λ_k^- (corresponding to K_-). This means

$$\begin{aligned} \mathscr{E}_k^+ &= \mathscr{E}(\Omega) - (2k+1+o(1))\, Z^{-1/3} K_+^{1/2} \\ \mathscr{E}_k^- &= \mathscr{E}(\Omega) - (2k+1+o(1))\, Z^{-1/3} K_-^{1/2} \end{aligned} \tag{II.47}$$

as $Z \to \infty$, uniformly for $k <$ any fixed integer K. Upon rescaling, (II.46) implies

$$(Z^{1/3}/\pi) \int [K_{\underset{(-)}{+}} x^2 - (2k+1)\, Z^{-1/3} K_{\underset{(-)}{+}}]_+ = k + \frac{1}{2}.$$

A simple continuity argument implies

$$(Z^{1/3}/\pi) \int [K_{\underset{(-)}{+}} x^2 - (2k+1+o(1))\, Z^{-1/3} K_{\pm}^{1/2}]_+^{1/2} = k + \frac{1}{2} + o(1), \tag{II.48}$$

as $Z \to \infty$, uniformly for $k <$ any fixed integer K. Equation (II.47), the definition of K, the fact that $\mathscr{E}_k^+ < \mathscr{E}_k < \mathscr{E}_k^-$, the accuracy of the quadratic approximation (see (II.41) and directly above it), and another simple continuity argument imply

$$(Z^{1/3}/\pi) \int [y(x) - \Omega/x^2 - \mathscr{E}_k]_+^{1/2}\, dx = k + \frac{1}{2} + o(1), \tag{II.49}$$

as $Z \to \infty$, uniformly for $k <$ any fixed integer $\bar{K}$.

Since $K_\pm$ are within $(1 \pm \text{const.}\, Z^{-1/36})$ of $p''(x_c)/2$ and hence of $c(\Omega)\, \Omega^{-3}$, condition (II.47) implies a uniform upper bound $\bar{K}$ on the number of eigenvalues $-\mathscr{E}_k$ which lie between $-\mathscr{E}(\Omega)$ and $-\mathscr{E}(\Omega) + 10MZ^{-1/3}\Omega^{-3/2}$. Hence (II.49) holds for the eigenvalues in question—in particular, for $\mathscr{E}_{K(Z,\Omega)}$. This takes care of the WKB Theorem and Estimate 3.

It remains to prove Estimates 1 and 2. We must calculate

$$\frac{d}{d\mathscr{E}} G(\Omega, \mathscr{E}) = (2\pi)^{-1} \int_{x_1}^{x_2} |p|^{-1/2}$$

and

$$\frac{d}{d\mathscr{E}} G(\Omega, \mathscr{E}) \left| \frac{d}{d\mathscr{E}} G(\Omega, \mathscr{E}) \right|^{-2}.$$

First, let us calculate the second derivative,

$$(2\pi) \frac{d^2}{d\mathscr{E}^2} G(\Omega, \mathscr{E}) = \lim_{h \to 0} h^{-1} \int (p_-(x)^{-1/2} - (p(x)+h)_-^{-1/2})\, dx,$$

where p_- is the absolute value of the negative part of p. Break this integral into two parts:

$$= \lim_{h \to 0} h^{-1} \int_{x_1+\varepsilon_1}^{x_2-\varepsilon_2} (p_-(x)^{-1/2} - (p(x)+h)_-^{-1/2})\, dx$$

$$+ \lim_{h \to 0} h^{-1} \int_{[x_1, x_1+\varepsilon_1] \cup [x_2-\varepsilon_2, x_2]} (p_-(x)^{-1/2} - (p(x)+h)_-^{-1/2})\, dx.$$

Since p_- is bounded from below by a positive number for $x \in [x_1+\varepsilon_1, x_2-\varepsilon_2]$, the first term converges to

$$\left(\frac{1}{2}\right) \int_{x_1+\varepsilon_1}^{x_2-\varepsilon_2} |p|^{-3/2}(x)\, dx.$$

Let us treat the part of the second term that is integrated over $[x_2-\varepsilon_2, x_2]$. In this case $p'(x_2)$ is positive and we need not worry about absolute value signs. This integral can be broken into two parts (forget about h^{-1} momentarily):

$$\int_{\{|p|<h\} \cap [x_2-\varepsilon_2, x_2]} |p|^{-1/2}\, dx + \int_{\{|p|<h\} \cap [x_2-\varepsilon_2, x_2]} (|p|^{-1/2} - |p+h|^{-1/2})\, dx.$$

As $h \to 0$, $p(x) = p'(x_2)(x-x_2)(1+O(h))$ and $\{|p|<h\} = \{|x-x_2| < hp'(x_2)^{-1}(1+O(h))\}$. Hence, the first term equals

$$2h^{1/2}p'(x_2)^{-1}(1+O(h)).$$

The second integral is more complicated. By getting a common denominator and factoring

$$[|p|^{-1/2} - |p+h|^{-1/2}] = -h|p|^{-3/2}(1+h/p)^{-1}(1+(1+h/p)^{1/2})^{-1}.$$

Let $t = p(x)/h$, $dt = (p'(x)/h)\, dx$. The second integral equals

$$-h \int_1^{|p(x_2-\varepsilon(x_2))|h^{-1}} t^{-3/2}(1-1/t)^{-1/2}(1+(1-1/t)^{1/2})^{-1} p'(x(t))^{-1}\, dt.$$

Since $p(x) = p'(x_2)(x-x_2) + O(p''(x_2)(x-x_2)^2)$, $p'(x(t)) = p'(x_2)\ p'(x(t)) = p'(x_2)(1+O(h+p''/p'^2))$. Hence, the integral equals

$$-h^{1/2}p'(x_2)^{-1} \int_1^{|p(x_2-\varepsilon(x_2))|h^{-1}} t^{-3/2}(1-1/t)^{-1/2}(1+(1-1/t)^{1/2})^{-1}\, dt$$

$$+ O(h^{3/2}p''p'^{-3}(x_2)) \int_1^{|p(x_2-\mathscr{E}(x_2))|h^{-1}} t^{-1/2}(1-1/t)^{-1/2}(1+(1-1/t)^{1/2})^{-1}\, dt.$$

The second of these two integrals equals

$$O(h^{3/2}p''p'^{-1}(x_2)\,p(x_2-\varepsilon(x_2))^{1/2}\,h^{-1/2})$$
$$= O(hp''(x_2)\,\varepsilon(x_2)^{1/2}\,p'(x_2)^{-5/2}).$$

To compute the first, change variables

$$v = t(1-(1-1/t)^{1/2})^2$$
$$dv = -v^{1/2}t^{-3/2}(1-1/t)^{-1/2}\,(1+(1-1/t)^{1/2})^{-1}\,dt.$$

The integral becomes

$$-h^{1/2}p'(x_2)^{-1}\int_{v(|p(x_2-\varepsilon(x_2))|h^{-1})}^{1} v^{-1/2}\,dv$$
$$= -2h^{1/2}p'(x_2)^{-1} + 2h^{1/2}p'(x_2)^{-1}\,v((p(x_2-\varepsilon(x_2))\,h^{-1}))^{1/2}.$$

For $h \to 0$, $v(|p(x_2-\varepsilon(x_2))|\,h^{-1}) = (1/4)(h\,|p(x_2-\varepsilon(x_2))|^{-1}) + O(h^{3/2})$. Hence, the integral equals

$$-2h^{1/2}p'(x_2)^{-1} + \frac{1}{2}\,hp'(x_2)^{-1}\,|p(x_2-\varepsilon(x_2))|^{-1/2}.$$

Adding up the contribution to $(d^2/d\mathscr{E}^2)\,G(\Omega, \mathscr{E})$, dividing by h, and letting $h \to 0$, we obtain

$$\frac{d^2}{d\mathscr{E}^2}\,G(\Omega, \mathscr{E}) = (1/2\pi)\int_{x_1+\varepsilon(x_1)}^{x_2-\varepsilon(x_2)} |p|^{-3/2}\,(x)\,dx$$
$$+\sum_{i=1}^{2}\,(1/4\pi)\,p'(x_i)^{-1}\,|p(x_i-\varepsilon_i)|^{-1/2}$$
$$+\sum_{i=1}^{2}\,\cdot\,O(p''(x_i)\,\varepsilon_i^{1/2}\,|p'(x_i)|^{-5/2}).$$

By choice of ε_i, these two terms equal const. $\sum_{i=1}^{2}|p'(x_i)|^{-3/2}\,\varepsilon_i^{-1/2}$ within a factor.

We now calculate

$$\frac{dG}{d\mathscr{E}}\,(\Omega, \mathscr{E}) = \text{const.}\int_{x_1}^{x_2} |p|^{-1/2}\,dx \tag{II.50}$$

$$\frac{d^2G}{d\mathscr{E}^2}\,(\Omega, \mathscr{E}) = \text{const.}\left\{\int_{x_1+\varepsilon_1}^{x_2-\varepsilon_2} |p|^{-3/2}\,dx + \sum_{i=1}^{2}\,|p'(x_i)|^{-3/2}\,\varepsilon_i^{-1/2}\right\}. \tag{II.51}$$

When $|\mathscr{E}-\mathscr{E}(\Omega)|<(c^3\bar{c}^{-2}10^{-6})\,\Omega^{-1}$, the quadratic approximation gives (II.50) within a small precentage error

$$\int_{x_1}^{x_2} |p|^{-1/2}\,dx \approx \int_{x_c-\sqrt{2(\mathscr{E}(\Omega)-\mathscr{E})\,p''(y_2)^{-1}}}^{x_c+\sqrt{2(\mathscr{E}(\Omega)-\mathscr{E})\,p''(y_2)^{-1}}} \left|\mathscr{E}-\mathscr{E}(\Omega)+\frac{1}{2}p''(y_2)(x-y_2)^2\right|^{-1/2} dx$$

$$\sqrt{2p''(x_c)^{-1}} \int_{-1}^{1} (1-u^2)^{-1/2}\,du.$$

Since $p''(y_c)=c(\Omega)\,\Omega^{-3}>c\Omega^{-3}$, this is

$$>\text{const.}\ \Omega^{-3/2}.$$

To obtain an upper bound on the integral in (II.51), multiply the value $|p|^{-3/2}\,(y_i\pm\varepsilon_i)$ by $|y_i-x_2|$. Then

$$\text{(II.51) is } <\text{const.} \sum_{i=1}^{2} \{|p'(y_i)|^{-3/2}\,\varepsilon_i^{-3/2}\,|y_1-x_2| + |p'(y_i)|^{-3/2}\,\varepsilon_i^{-1/2}\}.$$

By (II.19), these terms are all bounded by

$$\text{const.}\ \Omega^{3/2}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}.$$

Hence,

$$\left|\frac{d^2}{d\mathscr{E}^2}G(\Omega,\mathscr{E})\right| \left|\frac{d}{d\mathscr{E}}G(\Omega,\mathscr{E})\right|^{-2} < \text{const.}\ \Omega^{-3/2}(\mathscr{E}(\Omega)-\mathscr{E})^{-1}$$

in this case.

When $2\Omega+\text{const.}\ \Omega<x_2<\bar{x}$, $|p(x)|>\text{const.}\ (1/x-1/x_2)$. Hence,

$$\int_{x_1}^{x_2} |p|^{-1/2}\,dt > \text{const.} \int_{2}^{x_2} x^{1/2}dx > \text{const.}\ x_2^{3/2}.$$

To bound (II.51), consider separately $x<2\Omega$ and $x>2\Omega$. Since $x_1<2\Omega-\text{const.}\ \Omega$, $|p'(x_1)|>\text{const.}\ \Omega^{-2}$ $\varepsilon_1>(\text{small const.})\,\Omega$, and hence $|p(x_1+\varepsilon_1)|>\text{const.}\ \Omega^{-1}$. The minimum of $|p|$ over the interval $[x_1+\varepsilon_1, 2\Omega]$ occurs here. Hence,

$$\int_{x_1+\varepsilon_1}^{2\Omega} |p|^{-3/2} < \text{const.}\ \Omega^{5/2}.$$

Since $|p| > \text{const.}\, x^{-1}$ for $x < x_2 - \varepsilon_2$ (see (II.32)),

$$\int_{2\Omega}^{x_2-\varepsilon_2} |p|^{-3/2} < \text{const.}\, x_2^{5/2}.$$

The quantities at the endpoints are bounded by const. $\Omega^{5/2}$ and const. $x_2^{5/2}$, respectively. Hence,

$$\begin{aligned}\left|\frac{d^2}{d\mathscr{E}^2} G(\Omega, \mathscr{E})\right| \left|\frac{d}{d\mathscr{E}} G(\Omega, \mathscr{E})\right|^{-2} & \\ &\leqslant \text{const.}\, x_2^{-1/2} \\ &\leqslant \text{const.}\, \Omega^{-1/2}.\end{aligned}$$

When $x_2 > 2\bar{x}$, (II.34) implies that $|p(x) < \text{const.}\, |x_2^{-4} - x^{-4}|$ for $x \in (\bar{x}, y_2)$,

$$\int_{x_1}^{x_2} |p|^{-1/2}\, dx > \text{const.} \int_{\bar{x}}^{x_2} x^2 dx > \text{const.}\, x_2^3.$$

Also, $|p(x)| > \text{const.}\, x^{-4}$ when $x \in (\bar{x}, x_2 - \varepsilon_2)$,

$$|p| > \text{const.}\, x^{-1} \qquad \text{when} \quad x \in [x_c, \bar{x}],$$

and

$$|p| > \text{const.}\, \Omega^{-1} \qquad \text{when} \quad x \in [x_1 + \varepsilon_1, y_c].$$

Hence,

$$\begin{aligned}\int_{x_1+\varepsilon_1}^{x_2-\varepsilon_2} |p|^{-3/2}\, dx &= \int_{x_1+\varepsilon_1}^{x_c} |p|^{-3/2} + \int_{x_c}^{\bar{x}} |p|^{-3/2} + \int_{\bar{x}}^{x_2-\varepsilon_2} |p|^{-3/2} \\ &< \text{const.}\, (\Omega^{5/2} + \bar{x}^{5/2} + x_2^7).\end{aligned}$$

The terms in (II.51) at the left turning point are again bounded by $\Omega^{5/2}$ and those at the right turning point by x_2^7. (See (II.19) and (II.34).) The dominating quantity is x_2^7. Hence,

$$\left|\frac{d^2}{d\mathscr{E}^2} G(\Omega, \mathscr{E})\right| \left|\frac{d}{d\mathscr{E}} G(\Omega, \mathscr{E})\right|^{-2} < \text{const.}\, x_2 < \text{const.}\, \Omega^{-1/2}.$$

This completes the proof of Estimates 1 and 2.

Acknowledgments

This project would not have been possible without the expert, conscientious, and generous guidance of my thesis advisor, Charles Fefferman. He suggested the techniques and helped me around numerous difficulties. He is also one of the nicest people I know. I am permanently indebted.

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Printed in Belgium